

A11102 707022

NATL INST OF STANDARDS & TECH R.I.C.



A11102707022

Westley, Francis/Compilation of chemical
5 A30.W47 V1:1987 C.1 NSRDS 1987



NSRDS-NBS 73, Part 1

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards



Compilation of Chemical Kinetic Data for Combustion Chemistry.

**Part 1. Non-Aromatic C, H, O, N, and S
Containing Compounds.
(1971-1982)**

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³Located at Boulder, CO, with some elements at Gaithersburg, MD



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**Compilation of Chemical Kinetic
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**Part 1. Non-Aromatic C, H, O, N, and S
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Francis Westley, John T. Herron,
and R. J. Cvetanović

Chemical Kinetics Division
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Gaithersburg, MD 20899



U.S. DEPARTMENT OF COMMERCE, Clarence J. Brown, Acting Secretary
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, Director

Issued August 1987

For sale by the Superintendent of Documents, U.S. Government Printing Office
Washington, D.C. 20402

Library of Congress Cataloging-in-Publication Data

Westley, Francis.

Compilation of chemical kinetic data for combustion chemistry.

(NSRDS-NBS; 73, pt. 1-)

Includes bibliographies and index.

Contents: Pt. 1. Non-aromatic C, H, O, N, and S containing compounds (1971-1982)

1. Combustion—Tables. 2. Chemical reaction, Rate of—
Tables. I. Herron, John Thomas, 1931—
II. Cvetanović, R. J. III. Center for Chemical Physics (U.S.).
Chemical Kinetics Division. IV. Title.
V. Series: NSRDS-NBS ; 73, pt. 1, etc.
QC100.U573 no. 73 pt. 1, etc. 602'.18s 87-20244

[QD516]

[541.3'61'0212]

NSRDS-NBS 73, Part 1

Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.), 73, Part 1, 683 pages (Aug. 1987)

CODEN: NSRDAP

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Foreword

The National Standard Reference Data System was established in 1963 for the purpose of promoting the critical evaluation and dissemination of numerical data of the physical sciences. The program is coordinated by the Office of Standard Reference Data of the National Bureau of Standards but involves the efforts of many groups in universities, government laboratories, and private industry. The primary aim of the program is to provide compilations of critically evaluated physical and chemical property data. These tables are published in the *Journal of Physical and Chemical Reference Data*, in the NSRDS-NBS series of the National Bureau of Standards, and through other appropriate channels.

The task of critical evaluation is carried out in various data centers, each with a well-defined technical scope. A necessary preliminary step to the critical evaluation process is the retrieval from the world scientific literature of all papers falling within the scope of the center, followed by the extraction and organization of the numerical data contained in these papers. The present publication presents such a compilation of data prepared by the NBS Chemical Kinetics Data Center.

Further information on NSRDS and the publications which form the primary output of the program may be obtained by writing to the Office of Standard Reference Data, National Bureau of Standards, Gaithersburg, MD 20899.

DAVID R. LIDE, JR., *Director*
Office of Standard Reference Data

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Compilation of Chemical Kinetic Data for Combustion Chemistry. Part 1. Non-Aromatic C, H, O, N, and S Containing Compounds. (1971-1982)

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Chemical Kinetics Division, Center for Chemical Physics, National Bureau of Standards, Gaithersburg, MD. 20899

Chemical kinetics data for reactions of importance in combustion chemistry are compiled. Experimental, theoretical, evaluated, or estimated rate constants are given for reactions of O, O₂, O₃, H, H₂, OH, HO₂, H₂O, H₂O₂, N, N₂, N₃, NO, NO₂, NO₃, N₂O, N₂O₅, NH, NH₂, NH₃, NH=NH, NH₂=NH, NH₂=NH₂, HN₃, HNO, HONO, HONO₂, HO₂NO₂, NH₂O, NH₂O₂, S, S₂, SO, SO₂, SH, H₂S, and the aliphatic, alicyclic, and heterocyclic saturated and unsaturated C₁ to C₁₅ hydrocarbons, alcohols, aldehydes, ketones, thiols, ethers, peroxides, amines, amides, and their free radicals. The data were taken from the literature published between 1971 and 1982. Data previously issued in 1981 as NBSIR-81-2254, which covered the literature published from 1971 through 1977, are included. The data are reported as rate constants or in terms of the parameters *A*, *n*, and *B* of the extended Arrhenius expression $k = A(T/298)^n \times \exp(-B/T)$, where $B = E/R$. Data are given for 1931 reactions.

Key words: Arrhenius parameters; carbon; chemical kinetics; combustion; compilation; free radicals; gas phase; hydrocarbons; hydrogen; nitrogen; oxygen; rate of reaction; sulfur.

1. Introduction

1.1. Overview

This report provides a compilation of chemical kinetic data for use by modelers, experimentalists, and theoreticians interested in developing a detailed understanding of gas phase combustion processes involving fossil fuels. It is part of a larger effort to develop a comprehensive evaluated chemical kinetic data base, and is a necessary prelude to that effort. The present compilation covers the literature published between 1971 and 1982. It will be followed by subsequent compilations covering the literature published after 1982. These will then be updated approximately every three years.

The present work serves as the foundation for a set of evaluations on specific subsets of the larger data base. Those published or in preparation include:

- (1) "Chemical Kinetic Data Base for Combustion Chemistry. Part 1. Methane and Related Compounds", W. Tsang and R. F. Hampson, J. Phys. Chem. Ref. Data **15**, 1087 (1986).
- (2) "Chemical Kinetic Data Base for Combustion Chemistry. Part 2. Methanol", W. Tsang, J. Phys. Chem. Ref. Data **16**, (Sept. 1987).
- (3) "Chemical Kinetic Data Base for Combustion Chemistry. Part 3. Propane.", W. Tsang, J. Phys. Chem. Ref. Data (submitted).
- (4) "Chemical Kinetic Data Base for Combustion Chemistry. Part 4. Isobutane", W. Tsang (to be published).

- (5) "Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen O(³P) with Unsaturated Hydrocarbons", R. J. Cvetanović, J. Phys. Chem. Ref. Data **16**, 261 (1987).
- (6) "Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen O(³P) with Sulfur Containing Compounds", D. L. Singleton and R. J. Cvetanović (in preparation).
- (7) "Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen O(³P) with Saturated Organic Compounds", John T. Herron, J. Phys. Chem. Ref. Data (submitted).

1.2. Scope

Data are given for the reactions of aliphatic, alicyclic, and heterocyclic, saturated and unsaturated hydrocarbons and their derivatives, and for the reactions with inorganic species containing hydrogen, oxygen, nitrogen, and sulfur with themselves and with hydrocarbons and their derivatives. Not included are reactions involving aromatic species, halogens, halogen derivatives, ions, and, with few exceptions, excited states.

The data have been abstracted from the literature published between 1971 and 1982 inclusive. Some references to earlier work are included. All data published earlier in NBSIR-81-2254¹ are included.

Only publications containing numerical data have been abstracted. The abstracted data are either rate constants at some given temperature or the parameters *A*, *n*, and *B* of the extended Arrhenius expression $k = A(T/298)^n \exp(-B/T)$. Additional data on temperature range, pressure, nature of the third body, and the type of data (i. e., experimental, theoretical, estimated, etc.) are also provided.

1.3. Guide to the Table

1.3.1. General

The compilation is divided into two parts — a table of rate constants and a bibliography, which contains the references to the cited literature. The following describes the arrangement of the table with respect to contents and the order in which reactions are listed.

1.3.2. Arrangement of the Table

The table is arranged in eight columns. These list the chemical reaction, the data type, the temperature, the rate constant or the Arrhenius A factor, the n factor, the B factor where $B = E/R$, a term indicating the appropriate units for the rate constants, and an error factor. Other necessary information (such as the bibliographic citation, pressure and nature of bath gas, and notes on methodology or other factors) is given in the same column as the chemical reaction. A detailed description follows:

(1) Column 1 gives the chemical reaction. The names of the reactants given are the Chemical Abstracts Standard Names. Synonyms, enclosed in parentheses, are in some cases also given. Product names are given only in those cases in which the product is a bridged compound.

The bibliographic citation is given in the form of a Reference Code, which consists of the last two digits of the year of publication, followed by the first three letters of the names of the first and second author (if present) separated by a slash. An integer index is attached at the end when it is necessary to differentiate between otherwise identical Codes. This is illustrated by the Code 82 ATK/ASC2.

This column may also include information on the experimental method, analytical procedures, nature of the third body, pressure, identity of reference reaction in the case of relative rate measurements, or other comments.

(2) Column 2 indicates the type of data. The following abbreviations are used:

- EX = experimental
- RL = relative rate measurement
- RN = relative rate measurement normalized to an absolute value
- TH = theoretical
- CO = computed numerically
- ES = estimated
- SE = selected value in the literature
- RE = current NBS recommended value.

(3) Column 3 gives the temperature or temperature range.

(4) Column 4 lists the rate constant or the Arrhenius A factor, or the ratio of the rate constants.

(5) Column 5 gives the factor n for the extended Arrhenius expression $k = A(T/298)^n \exp(-B/T)$.

(6) Column 6 gives the parameter B for the extended Arrhenius expression $k = A(T/298)^n \exp(-B/T)$, where B is the Arrhenius activation energy divided by the gas constant, i.e., $B = E/R$. In the case of relative rate measurements the quantity reported is the difference $B - B(\text{ref})$, where $B(\text{ref})$ is the value of B for the reference reaction.

(7) Column 7 indicates the units of the rate constant or the Arrhenius A factor.

(8) Column 8 gives the error factor as reported in the original work.

1.3.3. Order of Reactions

The reactions are listed following the order of arrangement given in Table 1 of "The NBS Tables of Thermodynamic Properties".² In the present compilation the reactants contain any of the elements O, H, S, N, and C, and the order used is: O system, H-O system, S-O-H system, N-O-H-S system, and C-O-H-S-N system. Examples of the ordering of reactant species are given below:

- (1) O system: O, O₂, O₃
- (2) H-O system: H, H₂, OH, HO₂, H₂O, H₂O₂
- (3) S-O-H system: S, S₂, SO, SO₂, SO₃, SH, H₂S
- (4) N-O-H-S system: N, N₂, NO₂, NO₃, N₂O, N₂O₃, NH, etc.
- (5) C-O-H-S-N system: C, CO, CO₂, CH, CH₂, CH₃, CH₄, etc.

Index of reactions given below in Sec. 3 follows the same order of arrangement and can be used to find the page where a particular reaction is located in the Table of Chemical Kinetic Data for Combustion Chemistry. The reaction of ethylene with oxygen atoms, for example, is located at its proper place in the "O ATOM Reactions" at the beginning of the Index, since O atom (the O system) precedes ethylene (the C system).

1.3.4. Chemical Formulas and Nomenclature

Where possible, chemical formulas are written in semi-structural form. The following conventions are used:

- (1) For C₁ through C₅ saturated hydrocarbons and their O, S, and N derivatives, semi-structural formulas are used, e.g., (CH₃)₂CH₂CH₂ONO. Beyond C₅ the condensed forms are used, e.g., CH₃(CH₂)₈CH₂CN.
- (2) Unsaturated compounds are written to show the position of the double or triple bond, e.g., CH₂=C=CH₂.
- (3) The structures of all alicyclic and heterocyclic compounds are specified with figures in the text.

1.4. Acknowledgments

This work was supported by the Department of Energy, Division of Basic Energy Sciences and the Office of Standard Reference Data of the National Bureau of Standards. The authors are especially indebted to Mrs. Geraldine Zumwalt and Ms. Rhoda Levin for their attention to many details in the keyboarding, editing and preparation of the manuscript.

1.5. References to the Introduction

¹F. Westley, "Tables of Experimental Rate Constants for Chemical Reactions Occurring in Combustion (1971-1977)", NBSIR 81-2254, National Bureau of Standards, Gaithersburg, MD 20899 (1981).

²D. D. Wagman, W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, S. M. Bailey, K. L. Churney, and R. L. Nuttall, J. Phys. Chem. Ref. Data **11**, Suppl. 2 (1982).

2. Summary of Symbols and Units

Data Type Codes:

- EX (experimentally measured absolute value),
- RL (experimentally measured relative value),
- RN (RL normalized to absolute value),
- TH (theoretical value),
- DE (derived indirectly, e.g. using reverse rate and equilibrium constant, or computer simulation of a complex mechanism)
- CO (computed numerically),
- ES (estimated, by analogy etc),
- SE (selected in the literature as probable "best" value),
- RE (currently recommended value).

Type of excitation:

- † (vibrationally excited)
- * (electronically excited)

Decadic exponent notation: 1.2(11) (stands for 1.2×10^{11})

Temperature (T): in kelvins (K).

Arrhenius parameters are defined by

$$k = A(T/298)^n \exp(-B/T)$$

Unit Codes for k , $k/k(\text{ref})$, A , $A/A(\text{ref})$:

- 1 (s^{-1}),
- 2 ($\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$),
- 3 ($\text{cm}^6 \text{mol}^{-2} \text{s}^{-1}$),
- 1/1, 2/2 etc. (dimensionless),
- 2/1 ($\text{cm}^3 \text{mol}^{-1}$), etc.

($T/298$) and n (the exponent of T) are dimensionless.

Units for B , $B - B(\text{ref})$: kelvins (K). (Activation energy $E = R \times B$).

$k(\text{ref})$, $A(\text{ref})$ and $B(\text{ref})$ are the values for the "reference reaction" in relative rate determinations.

k err. factor: Estimated overall Uncertainty Factor. It multiplies and divides k or A to indicate approximate error limits. It does not imply that errors in k are necessarily lognormally distributed.

3. Index of Reactions

O ATOM Reactions:

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O + O (+ M)	51
O + O ₂ + O ₂	51
O + O ₂ (+ M)	51
O + O ₃	54
O(¹ D) + O ₃	55
O + H (+ M)	56
O + H ₂	56
O + D ₂	58
O(¹ D) + H ₂	58
O(¹ D) + D ₂	59
O + OH	59
O + HO ₂	60
O + H ₂ O	61
O(¹ D) + H ₂ O	61
O + H ₂ O ₂	63
O(¹ D) + H ₂ O ₂	63
O + SO (+ M)	63
O + SO ₂ (+ M)	63
O + SO ₃ (+ M)	64
O + S ₂ O	65
O + SH	65
O + H ₂ S	65
O + D ₂ S	66
O + N (+ M)	66
O + N ₂ (+ M)	66
O(¹ D) + N ₂ (+ M)	66
O + N ₃	67
O + NO (+ M)	67
O(¹ D) + NO	70
O + NO ₂ (+ M)	70
O(¹ D) + NO ₂	71
O + NO ₃	71
O + N ₂ O	71
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O + NS	75
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O + HONO	76
O + HONO ₂	76

O + HO ₂ NO ₂	76
O(¹ D) + CO	76
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O(¹ D) + CO ₂	78
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O + CH ₂	79
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O + CH ₃ NO ₂	88
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O + CH≡CH	89
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O + CH ₃ CH ₂	93
O + CH ₃ CH ₃	93
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O + CH=C=O	93
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O + cy-CH ₂ CH ₂ O (Ethylene epoxide)	94
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O + CH ₃ CH ₂ OH	95
O + CD ₃ CD ₂ OH	95
O + (CH ₃) ₂ O	96
O + cy-CH ₂ CH ₂ S (Ethylene episulfide)	96
O + CH ₃ CH ₂ SH	96
O + (CH ₃) ₂ S	97
O + CH ₃ SSCH ₃	97
O + CH ₃ CN	97
O + CH ₃ CH ₂ NH ₂	97

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O + CH ₃ CH ₂ ONO	98
O + O=C=C=C=O	98
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O + CH ₃ C≡CH	98
O + CH ₂ =C=CH ₂	99
O + CH ₃ CH=CH ₂	99
O(¹ D) + CH ₃ CH=CH ₂	100
O + cy-C ₃ H ₆	101
O + CH ₃ CH ₂ CH ₂	101
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O + CH ₃ C≡CCH ₃	104
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O + CH ₃ CH ₂ CH ₂ CH=CH ₂	111
O + (CH ₃) ₂ CHCH=CH ₂	111
O + (CH ₃) ₂ C=CHCH ₃	111
O(¹ D) + (CH ₃) ₂ C=CHCH ₃	111
O + cy-C ₅ H ₁₀ (Cyclopentane)	111
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O ₂ (¹ Δ _g) + cis-CH ₃ CH=CHCH ₃	120

$O_2(^1\Delta_g)$ + trans- $CH_3CH=CHCH_3$	120
$O_2(^1\Delta_g)$ + $(CH_3)_2C=CH_2$	120
$O_2(^1\Delta_g)$ + $CH_3CH_2CH_2CH_3$	120
$O_2(^1\Delta_g)$ + $CH_3C(O)OCH=CH_2$	120
$O_2(^1\Delta_g)$ + $CH_2=CHC(O)OCH_3$	120
O_2 + $(CH_3)_2CHCHO$	120
$O_2(^1\Delta_g)$ + $CH_3C(O)OCH_2CH_3$	121
$O_2(^1\Delta_g)$ + cy- C_5H_8 (Cyclopentene)	121
$O_2(^1\Delta_g)$ + $CH_3CH=C(CH_3)_2$	121
O_2 + $(CH_3)_2CHCH_2CH_3$	121
$O_2(^1\Delta_g)$ + cy- $C(CH_3)=CHCH=CHO$ (Furan, 2-methyl-)	121
$O_2(^1\Delta_g)$ + $CH_2=CHC(O)OCH_2CH_3$ (2-Propenoic acid ethyl ester) ...	121
$O_2(^1\Delta_g)$ + $CH_2=C(CH_3)C(O)OCH_3$ (2-Propenoic acid, 2-methyl-, methyl ester)	122
$O_2(^1\Delta_g)$ + cy- $(CH_2)_2CH=CHCH=CH$ (1,3-Cyclohexadiene)	122
$O_2(^1\Delta_g)$ + cy- $CH_2CH=CHCH_2CH=CH$ (1,4-Cyclohexadiene)	122
$O_2(^1\Delta_g)$ + cy- C_6H_{12} (Cyclohexene)	122
$O_2(^1\Delta_g)$ + cy- $(CH_2)_3CH=C(CH_3)$ (Cyclopentene, 1-methyl-)	122
$O_2(^1\Delta_g)$ + cy- $CH_2CH_2C(CH_3)=C(CH_3)$ (Cyclobutene, 1,2-dimethyl-) ..	123
$O_2(^1\Delta_g)$ + trans- $CH_3CH_2C(CH_3)=CHCH_3$	123
$O_2(^1\Delta_g)$ + $(CH_3)_2C=C(CH_3)_2$	123
O_2 + cy- C_6H_{12} (Cyclohexane)	123
$O_2(^1\Delta_g)$ + cy- C_6H_{12} (Cyclohexane)	123
$O_2(^1\Delta_g)$ + $CH_3(CH_2)_4CH_3$	123
$O_2(^1\Delta_g)$ + cy- $C(CH_3)=CHCH=C(CH_3)O$ (Furan, 2,5-dimethyl-)	124
$O_2(^1\Delta_g)$ + $(CH_3)_2CHCH_2OCH=CH_2$ (Propane, 1-(ethenyloxy)- 2-methyl-)	124
$O_2(^1\Delta_g)$ + $CH_3C(O)CH_2CH(CH_3)_2$ (2-Pentanone, 4-methyl-)	124
$O_2(^1\Delta_g)$ + $(CH_3)_2C=CHN(CH_3)_2$ (1-Propen-1-amine, N,N,2-trimethyl-)	124
$O_2(^1\Delta_g)$ + cy- $(CH_2)_4CH=C(CH_3)$ (Cyclohexene, 1-methyl-)	124
$O_2(^1\Delta_g)$ + cy- $(CH_2)_3C(CH_3)=C(CH_3)$ (Cyclopentene, 1,2-dimethyl-) ..	124
$O_2(^1\Delta_g)$ + $(CH_3)_2C=C(CH_3)CH_2CH_3$	125
O_2 + $CH_3(CH_2)_5CH_3$	125
$O_2(^1\Delta_g)$ + $CH_2=CHC(O)OCH_2CH_2CH_2CH_3$ (2-Propenoic acid butyl ester)	125
$O_2(^1\Delta_g)$ + $CH_3(CH_2)_5CHO$	125
$O_2(^1\Delta_g)$ + $CH_3C(O)OCH_2CH_2CH(CH_3)_2$ (1-Butanol, 3-methyl-, acetate)	125
O_2 + cy- $CH=CHCH=CHC(=CH_2)C(=CH_2)$ (1,3-Cyclohexadiene, 5,6-bis(methylene)-)	125
$O_2(^1\Delta_g)$ + cy- $(CH_2)_4C(CH_3)=C(CH_3)$ (Cyclohexene, 1,2-dimethyl-) ..	126
$O_2(^1\Delta_g)$ + $(CH_3)_2C=C(CH_3)CH_2CH_2CH_3$	126
O_2 + $(CH_3)_3CCH_2CH(CH_3)_2$ (Pentane, 2,2,4-trimethyl-)	126
$O_2(^1\Delta_g)$ + $C_2H_5OCH=C(C_2H_5)C_4H_9$ (1-Hexene, 1-ethoxy-2-ethyl-) ..	126

O_3 Reactions:

O_3 (+ M)	127
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$O_3 + SO$	127
$O_3(v=n) + SO$	127
$O_3 + SO_2$	128
$O_3 + H_2S$	128
$O_3 + NO$	128
$O_3 + NO^\dagger$	128
$O_3^\dagger + NO$	128
$O_3 + NO_2$	131
$O_3 + HONO$	131
$O_3 + CH_4$	132
$O_3 + HCHO$	132
$O_3 + CH_3ONO$	132
$O_3 + CH=CH$	132
$O_3 + CH_2=CH_2$	132
$O_3 + cis-CDH=CDH$	133
$O_3 + trans-CDH=CDH$	133
$O_3 + CD_2=CD_2$	133
$O_3 + CH_3CHO$	134
$O_3 + cy-CH_2CH_2S$ (Ethylene episulfide)	134
$O_3 + CH_3CH_2ONO$	134
$O_3 + CH_3C=CH$	134
$O_3 + CH_2=C=CH_2$	134
$O_3 + CH_3CH=CH_2$	134
$O_3 + CD_3CD=CD_2$	135
$O_3 + CH_2=CHCHO$	135
$O_3 + CH_3C(O)CHO$	135
$O_3 + CH_2=CHCN$	135
$O_3 + CH_3CH_2C=CH$	135
$O_3 + CH_3C=CCH_3$	135
$O_3 + CH_2=CHCH=CH_2$	136
$O_3 + CH_3CH_2CH=CH_2$	136
$O_3 + CH_3CH=CHCH_3$	136
$O_3 + cis-CH_3CH=CHCH_3$	136
$O_3 + trans-CH_3CH=CHCH_3$	136
$O_3 + (CH_3)_2C=CH_2$	137
$O_3 + CH_3CH=CHCHO$	137
$O_3 + CH_3C(O)CH=CH_2$	137
$O_3 + CH_2=C(CH_3)CHO$	138
$O_3 + cy-CH=CHCH=CHS$ (Thiophene)	138
$O_3 + CH_2=C(CH_3)CH=CH_2$	138
$O_3 + cy-C_5H_8$ (Cyclopentene)	138
$O_3 + CH_3CH_2CH_2CH=CH_2$	138
$O_3 + cis-CH_3CH_2CH=CHCH_3$	138
$O_3 + trans-CH_3CH_2CH=CHCH_3$	139
$O_3 + CH_3CH=C(CH_3)_2$	139
$O_3 + CH_3C(O)CH=CHCH_3$	139
$O_3 + cy-CH=CH(CH_2)_4$ (Cyclohexene)	139
$O_3 + CH_3CH_2CH_2CH_2CH=CH_2$	139
$O_3 + CH_3CH_2CH_2C(CH_3)=CH_2$	140

$O_3 + (CH_3)_2CHCH_2CH=CH_2$	140
$O_3 + cis-CH_3CH_2C(CH_3)=CHCH_3$	140
$O_3 + trans-CH_3CH_2C(CH_3)=CHCH_3$	140
$O_3 + (CH_3)_2C=C(CH_3)_2$	140
$O_3 + cy-C(O)CH=CH(CH_2)_3$ (2-Cyclohexen-1-one)	140
$O_3 + CH_3(CH_2)_4CH=CH_2$	140
$O_3 + cy-C_{10}H_{16}$ (Terpinolene)	141
$O_3 + bicy-C_{10}H_{16}$ (α -Pinene)	141
$O_3 + bicy-C_{10}H_{16}$ (β -Pinene)	141

H ATOM Reactions:

$H + O_2 (+ M)$	142
$H + O_2(^1\Delta_g)$	144
$D + O_2 (+ M)$	145
$H + O_3$	145
$H + H (+ M)$	146
$D + D (+ M)$	147
$H + H_2(v=1)$	148
$H + HD$	148
$H + HD(v=1)$	148
$H + D_2$	148
$H + D_2(v=1)$	148
$D + H_2$	148
$D + H_2(v=n)$	149
$D + HD$	149
$H + OH (+ M)$	149
$D + OH$	149
$H + OH + OH$	150
$H + OH + CO$	150
$H + HO_2$	150
$H + H_2O$	153
$H + H_2O_2$	153
$D + H_2O_2$	154
$H + SO_2$	154
$H + SH$	154
$H + H_2S$	154
$D + D_2S$	155
$H + N (+ M)$	155
$H + N_2$	155
$H + NO (+ M)$	155
$D + NO (+ M)$	157
$H + NO_2$	157
$H + N_2O$	157
$H + N_2O(v=3)$	158
$H + NH$	158
$H + NH_2 (+ M)$	158
$H + NH_3$	159
$H + NH_2NH$	159

H + NH ₂ NH ₂	159
H + HN ₃	159
H + HNO	159
H + HONO ₂	160
H + HO ₂ NO ₂	160
H + CO (+ M)	160
H + CO + OH	160
H + CO ₂	161
H + CH	161
H + CH ₂	161
H + CH ₃ (+ M)	161
H + CH ₄	162
D + CD ₄	163
H + CHO	163
H + HCHO	164
H + CH ₃ O	164
H + CD ₃ O	165
D + CH ₃ O	165
H + CH ₂ OH	165
H + CD ₂ OH	165
D + CH ₂ OD	166
H + CH ₃ OH	166
H + CD ₃ OH	166
H + CD ₃ OD	167
D + CH ₃ OH	167
H + CH ₃ OOH	167
D + CH ₃ OOH	167
H + COS	167
H + CH ₂ =N=N	168
H + CH ₃ NO ₂	168
H + CH ₃ ONO	168
H + CD ₃ ONO	168
H + CH=CH (+ M)	168
H + CD=CD (+ M)	169
D + CH=CH	170
D + CD=CD	170
H + CH ₂ =CH	171
H + CH ₂ =CH ₂ (+ M)	171
H + CH ₂ =CHD	173
H + CD ₂ =CD ₂ (+ M)	173
D + CH ₂ =CH ₂	174
D + CH ₂ =CHD	174
D + CD ₂ =CD ₂	174
H + CH ₃ CH ₂	175
H + CH ₃ CH ₃	175
H + CH ₂ =C=O	175
H + CH ₃ CO	176
H + CH ₃ CHO	176
H + CH ₂ CH ₂ OH	176

H + CH ₃ CH ₂ OH	176
H + (CH ₃) ₂ O	176
D + (CH ₃) ₂ O	177
H + CH ₃ OOCH ₃	177
H + cy-CH ₂ CH ₂ S (Ethylene episulfide)	177
H + (CH ₃) ₂ S	177
H + CH ₃ SSCH ₃	178
H + NCCN	178
H + O=C=C=C=O	178
H + CH ₃ C≡CH	178
H + CH ₂ =C=CH ₂	178
H + CH ₃ CH=CH ₂	179
H + CD ₃ CD=CD ₂	181
D + CH ₃ CH=CH ₂	181
D + CD ₃ CD=CD ₂	181
H + (CH ₃) ₂ CH	181
H + (CH ₃) ₂ CH [†]	182
H + CH ₃ CH ₂ CH ₃	182
H + CH ₂ =CHCHO	182
H + (CH ₃) ₂ CO	182
H + CH≡CC≡CH	183
H + CH ₂ =CHC≡CH	183
H + CH ₂ =CHCH=CH ₂ (+ M)	183
D + CH ₂ =CHCH=CH ₂	183
H + CH ₃ CH ₂ CH=CH ₂	184
D + CH ₃ CH ₂ CH=CH ₂	185
H + CH ₃ CH=CHCH ₃ (unspecified form)	185
H + cis-CH ₃ CH=CHCH ₃	185
D + cis-CH ₃ CH=CHCH ₃	186
H + trans-CH ₃ CH=CHCH ₃	186
D + trans-CH ₃ CH=CHCH ₃	187
H + (CH ₃) ₂ C=CH ₂ (+ M)	187
D + (CH ₃) ₂ C=CH ₂	188
H + (CH ₃) ₃ C	188
H + (CH ₃) ₃ C [†]	189
H + CH ₃ CH ₂ CH ₂ CH ₃	189
H + (CH ₃) ₃ CH	189
H + (CH ₃) ₃ COH	190
H + (CH ₃ CH ₂) ₂ O	190
H + cy-CH ₂ CH ₂ CH ₂ CH ₂ S (Thiophene, tetrahydro-)	190
H + CH ₃ CH ₂ CH ₂ CH ₂ SH	190
H + (CH ₃ CH ₂) ₂ S	190
H + CH ₃ CH ₂ SSCH ₂ CH ₃	191
H + CH ₃ CH ₂ CH ₂ CH=CH ₂	191
H + CH ₃ CH ₂ CH=CHCH ₃ (unspecified form)	191
H + CH ₃ CH ₂ C(CH ₃)=CH ₂	192
D + CH ₃ CH ₂ C(CH ₃)=CH ₂	192
H + (CH ₃) ₂ CHCH=CH ₂	192
D + (CH ₃) ₂ CHCH=CH ₂	192

H + CH ₃ CH=C(CH ₃) ₂	192
D + CH ₃ CH=C(CH ₃) ₂	193
H + CH ₃ CH ₂ CH ₂ CH ₂ CH ₃	193
H + (CH ₃) ₂ CHCH ₂ CH ₃	193
H + (CH ₃) ₄ C	193
H + (CH ₃) ₃ COCH ₃	194
H + CH ₃ CH ₂ CH ₂ C(CH ₃)=CH ₂	194
H + CH ₃ CH ₂ CH=C(CH ₃) ₂	194
H + CH ₃ CH ₂ C(CH ₃)=CHCH ₃	194
H + (CH ₃) ₂ C=C(CH ₃) ₂	195
D + (CH ₃) ₂ C=C(CH ₃) ₂	195
D + cy-C ₆ H ₁₂ (Cyclohexane)	195
H + CH ₃ (CH ₂) ₄ CH ₃	195
H + (CH ₃) ₂ CHCH(CH ₃) ₂	195
H + (CH ₃) ₂ CHN=NCH(CH ₃) ₂	196
H + (CH ₃) ₃ CCH(CH ₃) ₂	196
H + (CH ₃) ₃ CC(CH ₃) ₃	196

H₂ Reactions:

H ₂ (+ M)	197
D ₂ (+ M)	197
H ₂ + D ₂	197
HD + HD	197
H ₂ + NO	197
H ₂ (v>5) + NO	198
H ₂ + NO ₂	198
H ₂ + N ₂ O	198
H ₂ (X ¹ Σ _g ⁺) + C ₂ (X ¹ Σ _g ⁺)	198
H ₂ (X ¹ Σ _g ⁺) + C ₂ (a ³ Π _u)	199
D ₂ + C ₂ (a ³ Π _u)	199
H ₂ + C ₂ O	199
D ₂ + CH≡CH	199
H ₂ + C ₃	199
H ₂ + cy-CH ₂ CH ₂ CH=CHCH=CH (1,3-Cyclohexadiene)	199

OH RADICAL Reactions:

OH + O ₃	200
OH(v=n) + O ₃	200
OD(v=n) + O ₃	200
OH + H ₂	201
OH(v=1) + H ₂	202
OH(v=n) + H ₂ (v=1)	202
OH + HD	203
OH + D ₂	203
OD + H ₂	203
OD + D ₂	204
OH + OH (+ M)	204

OH + HO ₂	205
OH(v=9) + H ₂ O	207
OH + H ₂ O ₂	207
OH + S	208
OH + SO	208
OH + SO ₂ (+ M)	209
OH(v=9) + SO ₂	210
OH + H ₂ S	211
OH(v=9) + H ₂ S	211
OH + N ₂	212
OH(v=9) + N ₂	212
OH + NO (+ M)	212
OH(v=9) + NO	214
OH + NO ₂ (+ M)	214
OH + N ₂ O (+ M)	218
OH(v=9) + N ₂ O	218
OH + NH ₂	218
OH + NH ₃	219
OH + NH ₂ NH ₂	220
OH + HNO	220
OH + HONO	220
OH + HONO ₂	220
OH + HO ₂ NO ₂	222
OH + CO	222
OH + CO [†]	226
OD + CO	226
OH(v=1) + CO	227
OH(v=9) + CO ₂	227
OH + CH ₃	227
OH + CH ₄	228
OH(v=n) + CH ₄	229
OH + CDH ₃	229
OH + CD ₂ H ₂	229
OH + CD ₃ H	229
OH + CD ₄	230
OH + HCHO	230
OH + HCOOH	231
OH + CH ₃ OH	231
OH + CS ₂	231
OH + COS	232
OH(v=9) + COS	233
OH + CH ₃ SH	233
OH + CN	233
OH + HCN	234
OH + CH ₃ NH ₂	234
OH + NH ₂ NHCH ₃	234
OH + CH ₃ ONO	234
OH + CH ₃ NO ₂	234
OH + CH≡CH	235

OH + CH ₂ =CH ₂	236
OH + CD ₂ =CD ₂	238
OH + CH ₃ CH ₃	238
OH + CH ₂ =C=O	239
OH + CH ₃ CHO	239
OH + CH ₃ COOH	239
OH + CH ₃ CH ₂ OH	239
OH + (CH ₃) ₂ O	240
OH + (CH ₃) ₂ S	240
OH + CH ₃ SSCH ₃	240
OH + NCCN	241
OH + CH ₃ CN	241
OH + CH ₃ N=NCH ₃	241
OH + CH ₃ CH ₂ NH ₂	241
OH + (CH ₃) ₂ NH	241
OH + CH ₃ C(O)O ₂ NO ₂ (Peroxide, acetyl nitro-)	241
OH + CH ₃ CH ₂ ONO	242
OH + O=C=C=C=O	242
OH + CH ₃ C≡CH	242
OH + CH ₂ =C=CH ₂	242
OH + CH ₃ CH=CH ₂	242
OH + CD ₃ CH=CH ₂	244
OH + CH ₃ CD=CD ₂	244
OH + CD ₃ CD=CD ₂	244
OH + CH ₃ CH ₂ CH ₃	245
OH + CH ₂ =CHCHO	246
OH + CH ₃ C(O)CHO	246
OH + CH ₂ =CHCH ₂ OH	246
OH + CH ₂ =CHOCH ₃	247
OH + CH ₃ CH ₂ CHO	247
OH + (CH ₃) ₂ CO	247
OH + CH ₃ CH ₂ COOH	248
OH + CH ₃ C(O)OCH ₃	248
OH + CH ₃ CH ₂ CH ₂ OH	248
OH + (CH ₃) ₂ CHOH	248
OH + CH ₂ =CHCN	248
OH + CH ₃ CH ₂ CN	248
OH + (CH ₃) ₃ N	249
OH + CH ₃ CH ₂ CH ₂ ONO	249
OH + (CH ₃) ₂ CHONO ₂	249
OH + CH≡CC≡CH	249
OH + CH ₂ =CHCH=CH ₂	249
OH + CH ₃ CH ₂ CH=CH ₂	250
OH + cis-CH ₃ CH=CHCH ₃	250
OH + trans-CH ₃ CH=CHCH ₃	251
OH + (CH ₃) ₂ C=CH ₂	252
OH + cy-C ₄ H ₈ (Cyclobutane)	252
OH + CH ₃ CH ₂ CH ₂ CH ₃	252

OH + CD ₃ CD ₂ CD ₂ CD ₃	254
OD + CH ₃ CH ₂ CH ₂ CH ₃	254
OD + CD ₃ CD ₂ CD ₂ CD ₃	254
OH + (CH ₃) ₃ CH	254
OH + cy-CH=CHCH=CHO (Furan)	256
OH + CH ₃ CH=CHCHO	256
OH + CH ₃ C(O)CH=CH ₂	256
OH + CH ₂ =C(CH ₃)CHO	256
OH + CH ₃ CH ₂ CH ₂ CHO	256
OH + (CH ₃) ₂ CHCHO	257
OH + CH ₃ C(O)CH ₂ CH ₃	257
OH + CH ₃ CH ₂ CH ₂ COOH	258
OH + CH ₃ C(O)OCH ₂ CH ₃	258
OH + CH ₃ CH ₂ C(O)OCH ₃	258
OH + cy-CH ₂ CH ₂ CH ₂ CH ₂ O (Furan, tetrahydro-)	258
OH + CH ₃ CH ₂ CH ₂ CH ₂ OH	258
OH + (CH ₃ CH ₂) ₂ O	259
OH + (CH ₃) ₃ COOH	259
OH + cy-CH=CHCH=CHS (Thiophene)	259
OH + CH ₃ CH ₂ CH ₂ CH ₂ ONO	259
OH + CH ₃ CH ₂ CH(CH ₃)ONO	259
OH + (CH ₃) ₂ CHCH ₂ ONO	260
OH + (CH ₃) ₃ CONO	260
OH + CH ₃ CH ₂ CH ₂ CH ₂ ONO ₂	260
OH + CH ₃ CH ₂ CH(CH ₃)ONO ₂	260
OH + (CH ₃ CH ₂) ₂ NOH	261
OH + CH ₂ =C(CH ₃)CH=CH ₂	261
OH + CH ₃ CH ₂ CH ₂ CH=CH ₂	261
OH + CH ₃ CH ₂ CH=CHCH ₃	262
OH + cis-CH ₃ CH ₂ CH=CHCH ₃	262
OH + CH ₃ CH ₂ C(CH ₃)=CH ₂	262
OH + (CH ₃) ₂ CHCH=CH ₂	262
OH + (CH ₃) ₂ C=CHCH ₃	262
OH + cy-C ₅ H ₁₀ (Cyclopentane)	263
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH ₃	263
OH + (CH ₃) ₂ CHCH ₂ CH ₃	264
OH + (CH ₃) ₄ C	265
OH + CH ₃ CH ₂ CH ₂ CH ₂ CHO	265
OH + (CH ₃) ₂ CHCH ₂ CHO	266
OH + (CH ₃) ₃ CCHO	266
OH + CH ₃ C(O)CH ₂ CH ₂ CH ₃	267
OH + (CH ₃ CH ₂) ₂ CO	267
OH + CH ₃ C(O)OCH ₂ CH ₂ CH ₃ (Acetic acid propyl ester)	267
OH + CH ₃ CH ₂ C(O)OCH ₂ CH ₃ (Propanoic acid ethyl ester)	267
OH + CH ₃ CH ₂ CH ₂ CH(CH ₃)ONO ₂ (2-Pentanol nitrate)	267
OH + (CH ₃ CH ₂) ₂ CHONO ₂ (3-Pentanol nitrate)	268
OH + cy-(CH ₂) ₄ CH=CH (Cyclohexene)	268
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH=CH ₂ (1-Hexene)	268

OH + (CH ₃) ₃ CCH=CH ₂ (1-Butene, 3,3-dimethyl-)	268
OH + (CH ₃) ₂ C=C(CH ₃) ₂	269
OH + cy-C ₆ H ₁₂ (Cyclohexane)	269
OH + n-C ₆ H ₁₄	269
OH + (CH ₃) ₂ CHCH ₂ CH ₂ CH ₃ (Pentane, 2-methyl-)	270
OH + CH ₃ CH ₂ CH(CH ₃)CH ₂ CH ₃ (Pentane, 3-methyl-)	270
OH + (CH ₃) ₂ CHCH(CH ₃) ₂	271
OH + CH ₃ C(O)CH ₂ CH ₂ CH ₂ CH ₃ (2-Hexanone)	271
OH + CH ₃ CH ₂ C(O)CH ₂ CH ₂ CH ₃ (3-Hexanone)	272
OH + CH ₃ C(O)CH ₂ CH(CH ₃) ₂ (2-Pentanone, 4-methyl-)	272
OH + CH ₃ C(O)OCH(CH ₃)CH ₂ CH ₃ (Acetic acid 1-methylpropyl ester)	272
OH + CH ₃ CH ₂ CH ₂ OCH ₂ CH ₂ CH ₃ (di-n-Propyl ether)	273
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH(CH ₃)ONO ₂ (2-Hexanol nitrate)	273
OH + CH ₃ CH ₂ CH ₂ CH(CH ₂ CH ₃)ONO ₂ (3-Hexanol nitrate)	273
OH + cy-(CH ₂) ₄ CH=C(CH ₃) (Cyclohexene, 1-methyl-)	273
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH=CH ₂ (1-Heptene)	273
OH + n-C ₇ H ₁₆ (n-Heptane)	274
OH + (CH ₃) ₃ CCH(CH ₃) ₂ (Butane, 2,2,3-trimethyl-)	274
OH + (CH ₃) ₂ CHC(O)CH(CH ₃) ₂ (3-Pentanone, 2,4-dimethyl-)	275
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH(CH ₂ CH ₃)ONO ₂ (3-Heptanol nitrate)	275
OH + n-C ₈ H ₁₈ (n-Octane)	275
OH + CH ₃ (CH ₂) ₄ CH(CH ₂ CH ₃)ONO ₂ (3-Octanol nitrate)	275
OH + n-C ₉ H ₂₀ (n-Nonane)	276
OH + (CH ₃) ₂ CHCH ₂ C(O)CHCH ₂ (CH ₃) ₂ (4-Heptanone, 2,6-dimethyl-)	276
OH + bicy-C ₁₀ H ₁₆ (α-Pinene)	276
OH + bicy-C ₁₀ H ₁₆ (β-Pinene)	277
OH + n-C ₁₀ H ₂₂ (n-Decane)	277

HO₂ RADICAL Reactions:

HO ₂ + O ₃	277
HO ₂ + HO ₂ (+ M)	277
DO ₂ + DO ₂	280
HO ₂ + SO ₂ (+ M)	280
HO ₂ + NO (+ M)	280
DO ₂ + NO	282
HO ₂ + NO ₂ (+ M)	282
HO ₂ + N ₂ O	284
HO ₂ + NH ₂	284
HO ₂ + CO (+ M)	284
HO ₂ + CH ₄	285
HO ₂ + HCHO	285
HO ₂ + CH ₃ O ₂	286
HO ₂ + CH ₃ OH	286
HO ₂ + CH ₂ =CH ₂	286
HO ₂ + CH ₃ CH ₃	287
HO ₂ + CH ₃ CHO	287
HO ₂ + CH ₂ CH ₂ OH	287
HO ₂ + CH ₃ CH=CH ₂	287

$\text{HO}_2 + \text{CH}_3\text{CH}_2\text{CH}_3$	287
$\text{HO}_2 + \text{CH}_3\text{CH}_2\text{CHO}$	288
$\text{HO}_2 + \text{trans-CH}_3\text{CH=CHCH}_3$	288
$\text{HO}_2 + (\text{CH}_3)_3\text{CH}$	288
$\text{HO}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHO}$	289
$\text{HO}_2 + (\text{CH}_3)_2\text{CHCHO}$	289
$\text{HO}_2 + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$	289
$\text{HO}_2 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$ (Butane, 2,3-dimethyl-)	289

H_2O Reactions:

$\text{H}_2\text{O} (+ \text{M})$	289
$\text{D}_2\text{O} (+ \text{M})$	290
$\text{H}_2\text{O} + \text{SO}_3$	290
$\text{H}_2\text{O} + \text{NO}_2$	290
$\text{H}_2\text{O} + \text{NO}_2 + \text{NO}_2$	290
$\text{H}_2\text{O} + \text{N}_2\text{O}_3$	290
$\text{H}_2\text{O} + \text{N}_2\text{O}_4$	290
$\text{H}_2\text{O} + \text{N}_2\text{O}_5$	291

H_2O_2 Reactions:

$\text{H}_2\text{O}_2 (+ \text{M})$	291
$\text{H}_2\text{O}_2 + \text{NO}$	291
$\text{H}_2\text{O}_2 + \text{NO}_2$	291
$\text{H}_2\text{O}_2 + \text{N}_2\text{O}_5$	291
$\text{H}_2\text{O}_2 + \text{HONO}_2$	291

S_x ATOM Reactions:

$\text{S} + \text{O}_2$	292
$\text{S} + \text{O}_3$	292
$\text{S}(^1\text{D}) + \text{H}_2$	292
$\text{S} + \text{S} (+ \text{M})$	292
$\text{S} + \text{SH}$	292
$\text{S}(^1\text{D}) + \text{N}_2$	292
$\text{S}(^1\text{D}) + \text{NO}$	292
$\text{S} + \text{NO} (+ \text{M})$	293
$\text{S} + \text{NO}_2$	293
$\text{S}(^1\text{D}) + \text{N}_2\text{O}$	293
$\text{S}(^1\text{D}) + \text{CO}$	293
$\text{S}(^1\text{D}) + \text{CO}_2$	293
$\text{S}(^1\text{D}) + \text{CH}_4$	293
$\text{S} + \text{COS}$	294
$\text{S}(^1\text{D}) + \text{COS}$	294
$\text{S} + \text{CH}\equiv\text{CH}$	294
$\text{S}(^1\text{D}) + \text{CH}\equiv\text{CH}$	295
$\text{S} + \text{CD}\equiv\text{CD}$	295
$\text{S} + \text{CH}_2=\text{CH}_2$	295

S + CH ₂ =CD ₂	295
S + cis-CHD=CHD	296
S + CD ₂ =CD ₂	296
S(¹ D) + CH ₂ =CH ₂	296
S(¹ D) + CH ₃ CH ₃	296
S + cy-CH ₂ CH ₂ S (Ethylene episulfide)	296
S + CH ₃ C≡CH	297
S + CH ₃ CH=CH ₂	297
S + cy-CH(CH ₃)CH ₂ S (Thiirane, methyl-)	297
S + CH ₃ CH ₂ C≡CH	297
S + CH ₃ C≡CCH ₃	298
S + CH ₂ =CHCH=CH ₂	298
S + CH ₃ CH ₂ CH=CH ₂	298
S + cis-CH ₃ CH=CHCH ₃	299
S + trans-CH ₃ CH=CHCH ₃	299
S + (CH ₃) ₂ C=CH ₂	299
S + CH ₃ CH ₂ C≡CCH ₃	300
S + cy-C ₅ H ₈ (Cyclopentene)	300
S + CH ₃ CH ₂ C(CH ₃)=CH ₂	300
S + (CH ₃) ₂ C=CHCH ₃	300
S + (CH ₃) ₂ C=C(CH ₃) ₂	300
S ₂ (+ M)	301
S ₂ + S ₂ (+ M)	301

SO_x-COMPOUND Reactions:

SO (+ M)	301
SO + O ₂	301
SO + SO (+ M)	302
SO + SO ₃	302
SO + (SO) ₂ (Sulfur monoxide dimer)	302
SO + NO ₂	302
SO ₂ (+ M)	302
SO ₂ + SO ₂ (¹ B ₁)	303
SO ₂ + SO ₂ (³ B ₁)	303
SO ₂ + NO ₂	303
SO ₂ + NO ₃	304
SO ₂ + N ₂ O ₅	304
SO ₂ + CO	304
SO ₂ [*] + CO	304
SO ₂ ^{**} + CO	304
SO ₂ + CH≡CH	305
SO ₂ (³ B ₁) + CH≡CH	305
SO ₂ (³ B ₁) + cis-CH ₃ CH=CHCH ₃	305
SO ₂ (³ B ₁) + trans-CH ₃ CH=CHCH ₃	305
SO ₂ (¹ B ₁) + (CH ₃) ₃ CH	305
SO ₂ (³ B ₁) + (CH ₃) ₃ CH	305
SO ₂ (³ B ₁) + cis-CH ₃ CH ₂ CH=CHCH ₃	305
SO ₂ (³ B ₁) + trans-CH ₃ CH ₂ CH=CHCH ₃	306

SO ₃ (+ M)	306
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SH_x-COMPOUND Reactions:

SH + D ₂	306
SH + SH	306
SH + NO	306
H ₂ S (+ M)	306

N_x-COMPOUND Reactions:

N(⁴ S) + O ₂	307
N(² D) + O ₂	307
N(² P) + O ₂	307
N + O ₂ (¹ Δ _g)	307
N + O ₃	308
N(² D) + O ₃	308
N(² D) + H ₂	308
N + H ₂ (+ M)	308
N + OH	308
N(² D) + H ₂ O	309
N + SO ₃	309
N + N (+ M)	309
N + NO	309
N(² D) + NO	310
N(² P) + NO	310
N + NO ₂	310
N(² D) + N ₂ O	310
N(² P) + N ₂ O	311
N + HN ₃ (Hydrazoic acid)	311
N + NH ₂ NH ₂	311
N + C (+ M)	311
N(² D) + CO ₂	311
N + HCHO	311
N + CH ₃ OH	311
N + CH ₃ OD	312
N + CN	312
N + CH=CH	312
N + CH ₂ =CH ₂ (+ M)	312
N(² D) + CH ₂ =CH ₂	312
N(² P) + CH ₂ =CH ₂	313
N + CH ₃ CH ₂ OH	313
N + CH ₃ C=CH	313
N + CH ₃ CH=CH ₂	313
N + CH ₃ CH ₂ CH ₂ OH	313
N + (CH ₃) ₂ CHOH	313
N + CH ₂ =CHCH=CH ₂	314
N + CH ₃ CH ₂ CH=CH ₂	314
N + cis-CH ₃ CH=CHCH ₃	314

N + trans-CH ₃ CH=CHCH ₃	314
N + (CH ₃) ₂ C=CH ₂	314
N + NCC=CCN (2-Butynedinitrile)	314
N + (CH ₃) ₂ C=CHCH ₃	314
N ₂ (+ M)	315
N ₂ (A ³ Σ _u ⁺) + O ₂	315
N ₂ (A ³ Σ _u ⁺ , v=n) + O ₂	315
N ₃ + N ₃	315

N_xO_y-COMPOUND Reactions:

NO (+ M)	316
NO + O ₂ (¹ Δ _g)	316
NO + NO	316
NO + NO + NO	316
NO + NO + O ₂	316
NO + NO ₂ + H ₂ O	317
NO + NO ₃	317
NO + N ₂ O	317
NO + NH ₂	317
NO + NH ₃	317
NO + HNO	318
NO + HONO ₂	318
NO + C ₂ O	318
NO ₂ (+ M)	318
NO ₂ + NO ₂	318
NO ₂ + NO ₂ + CH ₃ OH	318
NO ₂ + NO ₂ + cy-CH ₂ CH ₂ O (Ethylene epoxide)	319
NO ₂ + NO ₂ + CH ₃ CH ₂ OH	319
NO ₂ + NO ₃ (+ M)	319
NO ₂ + NH ₃	320
NO ₂ + HONO	320
NO ₂ + CH ₄	320
NO ₂ + HCN	320
NO ₂ + CH ₂ =CH ₂	320
NO ₂ + CH ₃ CHO	320
NO ₂ + CH ₃ C=CH	321
NO ₂ + CH ₃ CH=CH ₂	321
NO ₂ + CH ₃ CH ₂ CH ₃	321
NO ₂ + CH ₃ CH ₂ CHO	321
NO ₂ + (CH ₃) ₂ CO	321
NO ₂ + CH ₂ =CHC=CH	321
NO ₂ + CH ₃ C=CCH ₃	321
NO ₂ + CH ₃ CH ₂ CH=CH ₂	321
NO ₂ + cis-CH ₃ CH=CHCH ₃	321
NO ₂ + trans-CH ₃ CH=CHCH ₃	322
NO ₂ + (CH ₃) ₂ C=CH ₂	322
NO ₂ + CH ₃ CH ₂ CH ₂ CHO	322
NO ₂ + CH ₃ CH ₂ N(↑O)=CHCH ₃ (Ethanamine, N-ethylidene-N-oxide-) ..	322

$\text{NO}_2 + (\text{CH}_3\text{CH}_2)_2\text{NOH}$ (Ethanamine, N-ethyl-N-hydroxy-)	322
$\text{NO}_2 + \text{CH}_2=\text{CHC}(\text{CH}_3)=\text{CH}_2$	322
$\text{NO}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$	323
$\text{NO}_3 + \text{NO}_3$	323
$\text{NO}_3 + \text{CH}_2=\text{CH}_2$	323
$\text{NO}_3 + \text{CH}_3\text{CHO}$	323
$\text{NO}_3 + \text{CH}_3\text{CH}=\text{CH}_2$	323
$\text{NO}_3 + \text{CD}_3\text{CD}=\text{CD}_2$	323
$\text{NO}_3 + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2$	324
$\text{NO}_3 + \text{cis-CH}_3\text{CH}=\text{CHCH}_3$	324
$\text{NO}_3 + \text{trans-CH}_3\text{CH}=\text{CHCH}_3$	324
$\text{NO}_3 + (\text{CH}_3)_2\text{C}=\text{CH}_2$	324
$\text{NO}_3 + \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2$	324
$\text{NO}_3 + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$	324
$\text{N}_2\text{O} (+ \text{M})$	324
$\text{N}_2\text{O}_5 (+ \text{M})$	326

N_xH_y -COMPOUND Reactions:

$\text{NH} + \text{O}_2$	327
$\text{NH} + \text{H}_2$	327
$\text{NH} + \text{N}_2 (+ \text{M})$	327
$\text{NH} + \text{NO}$	327
$\text{NH} + \text{NH}_2$	328
$\text{NH} + \text{NH}_3 (+ \text{M})$	328
$\text{NH}(\text{a}^1\Delta) + \text{HN}_3(\text{1A}')$	328
$\text{NH}(\text{b}^1\Sigma^+) + \text{NH}_3$	328
$\text{NH}(\text{a}^1\Delta) + \text{CH}_4$	329
$\text{NH}(\text{a}^1\Delta) + \text{CH}_2=\text{CH}_2$	329
$\text{NH}(\text{a}^1\Delta) + \text{cy-C}_3\text{H}_6$ (Cyclopropane)	329
$\text{NH}(\text{a}^1\Delta) + \text{cy-C}_6\text{H}_{12}$ (Cyclohexane)	329
$\text{NH}_2 + \text{O}_2 (+ \text{M})$	329
$\text{NH}_2 + \text{O}_3$	330
$\text{NH}_2 + \text{H}_2$	330
$\text{NH}_2 + \text{NO}$	331
$\text{NH}_2 + \text{NO}_2$	332
$\text{NH}_2 + \text{NH}_2 (+ \text{M})$	333
$\text{NH}_2 + \text{NH}_2\text{NH}_2$	333
$\text{NH}_2(\text{2A}_1) + \text{HN}_3(\text{1A}')$	334
$\text{NH}_2(\text{2A}_1) + \text{CH}_4$	334
$\text{NH}_2 + \text{HCONH}_2$ (Formamide)	334
$\text{NH}_2 + \text{CH}=\text{CH}$	334
$\text{NH}_2 + \text{CH}_2=\text{CH}_2$	334
$\text{NH}_2(\text{2A}_1) + \text{CH}_2=\text{CH}_2$	335
$\text{NH}_2 + \text{CH}_3\text{CH}_2$	335
$\text{NH}_2 + \text{CH}_3\text{CH}_3$	335
$\text{NH}_2 + \text{CH}_2=\text{C}=\text{CH}_2$	335
$\text{NH}_2 + \text{CH}_3\text{CH}=\text{CH}_2$	335
$\text{NH}_2 + \text{cy-C}_3\text{H}_6$ (Cyclopropane)	336

$\text{NH}_2(^2\text{A}_1) + \text{cy-C}_3\text{H}_6$ (Cyclopropane)	336
$\text{NH}_2 + (\text{CH}_3)_2\text{CH}$	336
$\text{NH}_2 + \text{CH}_3\text{CH}_2\text{CH}_3$	336
$\text{NH}_2 + \text{CH}_2=\text{CHCH}=\text{CH}_2$	337
$\text{NH}_2 + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2$	337
$\text{NH}_2 + \text{cis-CH}_3\text{CH}=\text{CHCH}_3$	337
$\text{NH}_2 + \text{trans-CH}_3\text{CH}=\text{CHCH}_3$	337
$\text{NH}_2 + (\text{CH}_3)\text{C}=\text{CH}_2$	337
$\text{NH}_2 + (\text{CH}_3)_3\text{C}$	337
$\text{NH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$	338
$\text{NH}_2 + (\text{CH}_3)_3\text{CH}$	338
$\text{NH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	338
$\text{NH}_3 (+ \text{M})$	338
$\text{NH}_3 + \text{HONO}$	339
$\text{NH}_3 + \text{CH}_2=\text{CHCN}$	339
$\text{NH}=\text{NH}$ (Diazene)	340
$\text{cis-NH}=\text{NH} + \text{CH}_2=\text{CHCH}=\text{CH}_2$	340
$\text{cis-NH}=\text{NH} + \text{cis-CH}_3\text{CH}=\text{CHCH}_3$	340
$\text{cis-NH}=\text{NH} + \text{trans-CH}_3\text{CH}=\text{CHCH}_3$	340
$\text{cis-NH}=\text{NH} + \text{cy-CH}_2\text{CH}_2\text{CH}=\text{CHCH}=\text{CH}$ (1,3-Cyclohexadiene)	340
$\text{cis-NH}=\text{NH} + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$	340
$\text{trans-NH}=\text{NH}$	341
$\text{trans-NH}=\text{NH} + \text{cis-NH}=\text{NH}$	341
$\text{trans-ND}=\text{ND}$	341
$\text{trans-ND}=\text{ND} + \text{cis-ND}=\text{ND}$	341
$\text{NH}_2\text{NH} + \text{NH}_2\text{NH}$	341
$\text{NH}_2\text{NH}_2 (+ \text{M})$	341
$\text{HN}_3 (+ \text{M})$	341

NH_xO_y -COMPOUND Reactions:

$\text{HNO} + \text{HNO}$	342
$\text{DNO} + \text{DNO}$	342
$\text{HONO} (+ \text{M})$	342
$\text{HONO}^\dagger$	342
$\text{HONO} + \text{O}_3$	343
$\text{HONO} + \text{HONO}$	343
$\text{HONO} + \text{HONO}_2$	343
$\text{HONO}_2 (+ \text{M})$	343
$\text{HO}_2\text{NO}_2 (+ \text{M})$	344
NH_2O	344
$\text{NH}_2\text{O} + \text{O}_3$	344
$\text{NH}_2\text{O}_2^\dagger$ (Aminodioxy)	344

C ATOM Reactions:

$\text{C} + \text{O}_2$	345
$\text{C}(2^1\text{D}_2) (+ \text{M})$	345
$\text{C}(2^1\text{D}_2) + \text{H}_2$	345

C + H ₂ (+ M)	345
C + H ₂ O	345
C + N ₂ (+ M)	345
C + NO	346
C + N ₂ O	346
C + C (+ M)	346
C + CO (+ M)	346
C + CO ₂	346
C + CH ₂	346
C + CH ₄	347
C + CN	347
C + O=C=C=C=O	347
C(¹ S ₀) + O=C=C=C=O	347

CO_x-COMPOUND Reactions:

CO + O ₂	347
CO + O ₃	347
CO + SO ₂ (³ B ₁)	347
CO + NO ₂	347
CO + NO ₂ (² B ₂)	348
CO + N ₂ O	348
CO ₂ (+ M)	348
CO ₂ + C ₂ O	349

CH RADICAL Reactions:

CH + O ₂	349
CH + H ₂	349
CH + H ₂ O	350
CH + N ₂ (+ M)	350
CH + NO	350
CH + NO ₂	351
CH + N ₂ O	351
CH + NH ₃	351
CH + CO	351
CH + CO ₂	352
CH + CH ₂	352
CH + CH ₄	352
CH + CH=CH	352
CH + CH ₂ =CH ₂	353
CH + CH ₃ CH ₃	353
CH + CH ₃ C≡CH	354
CH + cy-C ₃ H ₆ (Cyclopropane)	354
CH + CH ₃ CH ₂ CH ₃	354
CH + CH ₃ CH ₂ CH ₂ CH ₃ (n-Butane)	354
CH + cy-C ₆ H ₁₂ (Cyclohexane)	354

CH₂ Reactions:

CH ₂ (X ³ B ₁) + O ₂	354
CH ₂ (a ¹ A ₁) + O ₂	355
CH ₂ (X ³ B ₁) + H ₂	355
CH ₂ (a ¹ B ₁) + H ₂	355
CH ₂ (¹ A ₁) + H ₂ O	355
CH ₂ (X ³ B ₁) + N ₂	355
CH ₂ (X ³ B ₁) + NO	356
CH ₂ (a ¹ A ₁) + NO	356
CH ₂ (X ³ B ₁) + CO	356
CH ₂ (a ¹ A ₁) + CO	356
CH ₂ (X ³ B ₁) + CO ₂	356
CH ₂ (X ³ B ₁) + CH ₃	356
CH ₂ (X ³ B ₁) + CH ₄	357
CH ₂ (X ³ B ₁) + CH ₂ =N=N (Methane, diazo-)	357
CH ₂ (¹ A ₁) + CH ₂ =N=N (Methane, diazo-)	357
CH ₂ (X ³ B ₁) + CH=CH	357
CH ₂ (X ³ B ₁) + CH ₃ CH ₃	358
CH ₂ (a ¹ A ₁) + CH ₂ =C=O (Ketene)	358
CH ₂ (a ¹ B ₁) + CH ₂ =C=O (Ketene)	358
CD ₂ + CD ₂ =C=O (Ketene-d ₂)	359
CH ₂ (X ³ B ₁) + CH ₃ CH ₂ CH ₃	359
CH ₂ (a ¹ A ₁) + CH ₃ CH ₂ CH ₃	360
CH ₂ (a ¹ A ₁) + CH ₂ =CHCH=CH ₂ (1,3-Butadiene)	360
CH ₂ (X ³ B ₁) + CH ₃ CH ₂ CH ₂ CH ₃ (n-Butane)	360
CH ₂ (a ¹ A ₁) + CH ₃ CH ₂ CH ₂ CH ₃ (n-Butane)	361
CH ₂ (X ³ B ₁) + (CH ₃) ₃ CH (Propane, 2-methyl-)	361
CH ₂ (a ¹ A ₁) + CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ (n-Pentane)	362
CD ₂ + (CH ₃) ₄ C (Propane, 2,2-dimethyl-)	362

CH₃ RADICAL Reactions:

CH ₃ (+ M)	362
CH ₃ + O ₂ (+ M)	362
CD ₃ + O ₂	365
CH ₃ + O ₃	365
CH ₃ + H ₂	366
CH ₃ [*] + H ₂	366
CH ₃ + HD	366
CH ₃ + D ₂	366
CH ₃ [*] + D ₂	366
CD ₃ + H ₂	366
CD ₃ [*] + H ₂	367
CD ₃ + HD	367
CD ₃ [*] + D ₂	367
CH ₃ + SO ₂ (+ M)	367
CH ₃ + NO (+ M)	367

CH ₃ + NO ₂ (+ M)	368
CH ₃ + N ₂ O	368
CH ₃ + CO (+ M)	368
CH ₃ + CH ₃ (+ M)	369
CH ₃ * + CH ₃	371
CD ₃ + CD ₃ (+ M)	371
CH ₃ + CH ₄	372
CH ₃ + CHO	372
CH ₃ + HCHO (Formaldehyde)	372
CH ₃ + CH ₃ O (Methoxy)	372
CH ₃ + CH ₃ O ₂ (Methyldioxy)	373
CD ₃ + COS	373
CH ₃ + CH ₃ N=NH (Diazene, methyl-)	373
CH ₃ + CH ₃ NO ₂ (Methane, nitro-)	373
CH ₃ + CH=CH	373
CH ₃ + CH ₂ =CH ₂	373
CH ₃ + CH ₃ CH ₂	374
CH ₃ + CH ₃ CH ₃	374
CH ₃ + CH ₃ CO (Acetyl)	375
CD ₃ + CD ₃ CO (Acetyl-d ₃)	375
CH ₃ + CH ₃ CHO (Acetaldehyde)	376
CH ₃ + CH ₃ CDO (Acetaldehyde-1-d)	376
CH ₃ + HC(O)OCH ₃ (Formic acid methyl ester)	376
CD ₃ + HC(O)OCH ₃ (Formic acid methyl ester)	376
CD ₃ + DC(O)OCH ₃ (Formic-d acid methyl ester)	376
CH ₃ + (CH ₃) ₂ O (Dimethyl ether)	377
CH ₃ + cy-CH ₂ CH ₂ S (Thiirane; Ethylene episulfide)	377
CD ₃ + cy-CH ₂ CH ₂ S (Thiirane; Ethylene episulfide)	377
CH ₃ + (CH ₃) ₂ S (Dimethyl sulfide)	377
CH ₃ + CH ₃ N=NCH ₃ (Azomethane)	378
CD ₃ + CH ₃ N=NCH ₃ (Azomethane)	378
CH ₃ + CH ₂ =C=CH ₂ (Allene)	378
CH ₃ + (CH ₃) ₂ CH (Isopropyl)	378
CH ₃ + CH ₃ CH ₂ CH ₃ (Propane)	378
CH ₃ + CH ₃ C(O)CHO (Propanal, 2-oxo-)	379
CH ₃ + (CH ₃) ₂ CO (2-Propanone)	379
CH ₃ + (CD ₃) ₂ CO (2-Propanone-1,1,1,3,3,3-d ₆)	379
CD ₃ + (CD ₃) ₂ CO (2-Propanone-1,1,1,3,3,3-d ₆)	379
CH ₃ + CH ₃ C(O)OCH ₃ (Methyl acetate)	380
CH ₃ + CH ₃ C(O)OCD ₃ (Methyl-d ₃ acetate)	380
CH ₃ + CD ₃ C(O)OCH ₃ (Methyl acetate-d ₃)	380
CH ₃ + cy-CH(CH ₃)CH ₂ S (Thiirane, methyl-)	380
CH ₃ + (CH ₃) ₂ CHNO ₂ (Propane, 2-nitro-)	381
CH ₃ + CH ₂ C(CH ₃)=CH ₂ (2-Propenyl, 2-methyl-)	381
CH ₃ + trans-CH ₃ CH=CHCH ₃	381
CH ₃ + (CH ₃) ₂ C=CH ₂	381
CH ₃ + (CH ₃) ₃ C (tert-Butyl)	381
CH ₃ + CH ₃ CH ₂ CH ₂ CH ₃ (n-Butane)	381
CH ₃ + (CH ₃) ₃ CH (i-Butane)	382

CH ₃ + CH ₃ C(O)C(O)CH ₃ (Biacetyl)	382
CH ₃ + CD ₃ C(O)C(O)CD ₃ (Biacetyl-d ₆)	383
CD ₃ + CH ₃ C(O)C(O)CH ₃ (Biacetyl)	383
CD ₃ + CD ₂ HC(O)C(O)CD ₃ (Biacetyl-d ₅)	383
CD ₃ + CD ₃ C(O)C(O)CD ₃ (Biacetyl-d ₆)	383
CH ₃ + CH ₃ C(O)CH ₂ CH ₃ (2-Butanone)	384
CH ₃ + CD ₃ C(O)CD ₂ CH ₃ (2-Butanone-1,1,1,3,3-d ₅)	384
CH ₃ + CH ₃ CH ₂ CH ₂ CH=CH ₂ (1-Pentene)	384
CH ₃ + CH ₃ CH ₂ CH=CHCH ₃ (2-Pentene) (Unspecified form)	384
CH ₃ + CH ₃ CH=C(CH ₃) ₂ (2-Butene, 2-methyl-)	385
CH ₃ + CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ (n-Pentyl)	385
CH ₃ + CH ₃ CH ₂ CH ₂ CHCH ₃ (Butyl, 1-methyl-)	385
CH ₃ + (CH ₃) ₄ C (Neopentane)	385
CH ₃ + CH ₃ C(O)C(O)CH ₂ CH ₃ (2,3-Pentanedione)	386
CH ₃ + CH ₃ CD ₂ C(O)CD ₂ CH ₃ (3-Pentanone-2,2,4,4-d ₄)	386
CH ₃ + CH ₃ CH ₂ CH ₂ C(CH ₃)=CH ₂ (1-Pentene, 2-methyl-)	386
CH ₃ + CH ₃ CH ₂ CH=C(CH ₃) ₂ (2-Pentene, 2-methyl-)	386
CH ₃ + CH ₃ (CH ₂) ₄ CH ₃ (n-Hexane)	387
CH ₃ + (CH ₃) ₂ CHCH(CH ₃) ₂ (Butane, 2,3-dimethyl-)	387
CH ₃ + CH ₃ C(O)CH ₂ CH ₂ C(O)CH ₃ (2,5-Hexanedione)	387
CH ₃ + (CH ₃) ₃ COOC(CH ₃) ₃ (Peroxide, bis(1,1-dimethylethyl)-)	387

CH₄ Reactions:

CH ₄ (+ M)	388
CD ₄ (+ M)	389

CH_xO_y-COMPOUND Reactions:

CHO (+ M)	389
CHO + O ₂ (+ M)	389
CHO + NO	390
CHO + NO ₂	391
CHO + CHO	391
CHO + CH ₃ CH ₂ CH ₂ (n-Propyl)	392
CHO + CH ₃ CH ₂ CH ₂ CHOH (Butyl, 1-hydroxy-)	392
HCHO* (or HC(:)OH) (Formaldehyde (or Methylene, hydroxy-))	392
HCHO (+ M)	392
DCDO (+ M)	393
HCOOH (+ M)	393
HCOOH + HCOOH (Formic acid)	394
CH ₃ O (+ M)	394
CH ₃ O*	394
CH ₃ O + O ₂	394
CH ₃ O + O ₃	395
CH ₃ O + NO	395
CH ₃ O + NO ₂	396
CH ₃ O + N ₂ O	397
CH ₃ O + NH ₃	397

CH ₃ O + CO	397
CH ₃ O + CH ₄	397
CH ₃ O + CH ₃ O	397
CD ₃ O + CD ₃ O	398
CH ₃ O + CH ₃ OH	398
CH ₃ O + CH ₂ =CH ₂	398
CH ₃ O + CH ₃ CO (Acetyl)	398
CH ₃ O + CH ₃ CHO	398
CH ₃ O + CH ₃ OOCH ₃ (Peroxide, dimethyl-)	399
CH ₃ O + (CH ₃) ₃ C (tert-Butyl)	399
CH ₃ O + (CH ₃) ₃ CH	399
CH ₃ O + CH ₃ CH ₂ CH=CH ₂ (1-Butene)	399
CH ₃ O + (CH ₃) ₃ COOH (t-Butyl hydroperoxide)	399
CH ₃ O + (CH ₃) ₂ CHCH(CH ₃) ₂ (Butane, 2,3-dimethyl-)	399
CH ₂ OH (+ M)	399
CH ₂ OH + O ₂	400
CH ₂ OH + H ₂ O	400
CH ₂ OH + H ₂ O ₂	400
CH ₃ O ₂ + O ₃	400
CH ₃ O ₂ + SO ₂	400
CH ₃ O ₂ + NO	401
CH ₃ O ₂ + NO ₂	403
CH ₃ O ₂ + CO	403
CH ₃ O ₂ + HCHO	404
CH ₃ O ₂ + CH ₃ O ₂	404
CD ₃ O ₂ + CD ₃ O ₂	406
CH ₃ O ₂ + CH ₂ =CH ₂	406
CH ₃ O ₂ + CH ₃ C(O)OO (Ethyldioxy, 1-oxo-)	406
CH ₃ O ₂ + CH ₃ N=NCH ₃ (Azomethane)	406
CH ₃ O ₂ + (CH ₃) ₂ CHO ₂ (Ethyldioxy, 1-methyl-)	407
CH ₃ O ₂ + (CH ₃) ₂ C=CH ₂	407
CH ₃ O ₂ + (CH ₃) ₃ CO ₂ (Ethyldioxy, 1,1-dimethyl-)	407
CH ₃ O ₂ + CH ₂ =C(CH ₃)CH ₂ CH ₃ (1-Butene, 2-methyl-)	407
CH ₃ O ₂ + (CH ₃) ₂ C=CHCH ₃ (2-Butene, 2-methyl-)	407
CH ₃ O ₂ + (CH ₃) ₂ C=C(CH ₃) ₂ (2-Butene, 2,3-dimethyl-)	408
CH ₃ O ₂ + (CH ₃) ₂ CHCH(CH ₃) ₂ (Butane, 2,3-dimethyl-)	408
CH ₃ O ₂ + (CH ₃) ₂ CHC(OO·)(CH ₃) ₂ (Propyldioxy, 1,1,3-trimethyl-)	408
HOCH ₂ O + O ₂	408
HOCH ₂ O + NO	408
HOCH ₂ O ₂	409
HOCH ₂ O ₂ + NO	409
HOCH ₂ O ₂ + HOCH ₂ O ₂ (Methyldioxy, hydroxy-)	409
CH ₃ OH (+ M)	409

CS_x-COMPOUND Reactions:

CS ₂ (+ M)	410
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COS Reactions:

COS (+ M)	410
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CH_xS_y-COMPOUND Reactions:

CH ₃ S + CH ₃ S	410
CH ₃ S + cy-CH ₂ CH ₂ S (Thiirane; Ethylene episulfide)	410

CN RADICAL Reactions:

CN (+ M)	411
CN(v=n) + O ₂	411
CN + H ₂	411
CN(v=n) + NO(v'=0)	412
CN(v=n) + NO (+ M)	412
CN + CO ₂	412
CN(v=n) + CH ₄	412
CN + CD ₄	413
CN + COS	413
CN(v=n) + CH≡CH	413
CN + CH ₂ =CH ₂	413
CN + CH ₃ CH ₃	413
CN + NCCN	414
CN + CH ₃ CH=CH ₂	414
CN + CH ₃ CH ₂ CH ₃	414
CN + CH ₂ =CHCH=CH ₂	414

CON-COMPOUND Reactions:

NCO + O ₂	414
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CH_xN_y-COMPOUND Reactions:

HCN (+ M)	414
CH ₃ NH ₂ (+ M)	414
CH ₃ N=N (Diazenyl, methyl-)	415
CH ₃ NHNH ₂ (Hydrazine, methyl-)	415

CH_xO_yN_z-COMPOUND Reactions:

NH ₂ CO (+ M)	415
NH ₂ CO + NH ₂ CO (Amidogen, formyl-)	415
CH ₃ NO† (Methane, nitroso-)	415
CH ₃ ONO (+ M)	415
CH ₃ NO ₂ (+ M)	416
CH ₃ ONO ₂	416

CH ₃ O ₂ NO ₂ (+ M) (Peroxynitric acid methyl ester)	416
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C₂ (Carbon dimer) Reactions:

C ₂ (X ¹ Σ _g ⁺ = A ³ Π _g) (+ M)	417
C ₂ (X ¹ Σ _g ⁺) + O ₂	417
C ₂ (a ³ Π _u) + O ₂	417
C ₂ (X ¹ Σ _g ⁺) + H ₂ O	418
C ₂ (a ³ Π _u) + H ₂ O	418
C ₂ (X ¹ Σ _g ⁺) + N ₂	418
C ₂ (a ³ Π _u) + N ₂	418
C ₂ (X ¹ Σ _g ⁺) + NO	418
C ₂ (a ³ Π _u) + NO	419
C ₂ (X ¹ Σ _g ⁺) + CO ₂	419
C ₂ (a ³ Π _u) + CO ₂	419
C ₂ (X ¹ Σ _g ⁺) + CH ₄	419
C ₂ (a ³ Π _u) + CH ₄	420
C ₂ (X ¹ Σ _g ⁺) + CH≡CH	420
C ₂ (a ³ Π _u) + CH≡CH	420
C ₂ (X ¹ Σ _g ⁺) + CH ₂ =CH ₂	420
C ₂ (a ³ Π _u) + CH ₂ =CH ₂	421
C ₂ (X ¹ Σ _g ⁺) + CH ₃ CH ₃	421
C ₂ (a ³ Π _u) + CH ₃ CH ₃	421
C ₂ (X ¹ Σ _g ⁺) + CH ₂ =CHCN	421
C ₂ (a ³ Π _u) + CH ₂ =CHCN	421
C ₂ (X ¹ Σ _g ⁺) + CH ₂ =C=CH ₂	421
C ₂ (a ³ Π _u) + CH ₂ =C=CH ₂	422
C ₂ (X ¹ Σ _g ⁺) + CH ₃ CH ₂ CH ₃	422
C ₂ (a ³ Π _u) + CH ₃ CH ₂ CH ₃	422
C ₂ (a ³ Π _u) + CH ₃ CH ₂ CH ₂ CH ₃	422

C₂O Reactions:

C ₂ O + CH≡CH	422
C ₂ O + CH ₂ =CH ₂	422
C ₂ O + (CH ₃) ₂ C=CH ₂	423

C₂H_x-COMPOUND Reactions:

CH≡C (+ M)	423
CH≡C + O ₂	423
CH≡C + H ₂	423
CH≡C + CH ₄	424
CH≡C + CH≡CH	424
CH≡C + CD≡CD	425
CH≡C + CH ₃ CH ₃	425
CH≡C + CD ₃ CD ₃	425
CH≡C + CH ₃ C≡CH	425
CH≡C + CH≡CC≡CH	425

$\text{CH}=\text{C} + \text{CH}_2=\text{CHC}=\text{CH}$ (1-Buten-3-yne)	426
$\text{CH}=\text{C} + (\text{CH}_3)_4\text{C}$	426
$\text{CH}=\text{CH} (+ \text{M})$	426
$\text{CH}=\text{CH} + \text{CH}=\text{CH}$	427
$\text{CH}=\text{CH} + \text{cy-CH}=\text{CHCH}=\text{CHCH}_2$ (1,3-Cyclopentadiene)	427
$\text{CH}=\text{CH} + \text{cy-CH}_2\text{CH}_2\text{CH}=\text{CHCH}=\text{CH}$ (1,3-Cyclohexadiene)	427
$\text{CH}_2=\text{CH} (+ \text{M})$	428
$\text{CH}_2=\text{CH} + \text{CH}=\text{CH}$	428
$\text{CH}_2=\text{CH} + \text{CH}_2=\text{CH}$	428
$\text{CH}_2=\text{CH} + \text{CH}_3\text{CH}_2$	428
$\text{CH}_2=\text{CH}_2 (+ \text{M})$	428
$\text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{CH}_2$	429
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2$	429
$\text{CH}_2=\text{CH}_2 + \text{cis-CH}_3\text{CH}=\text{CHCH}_3$	429
$\text{CH}_2=\text{CH}_2 + \text{trans-CH}_3\text{CH}=\text{CHCH}_3$	429
$\text{CH}_2=\text{CH}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2$	430
$\text{CH}_2=\text{CH}_2 + \text{cy-CH}=\text{CHCH}=\text{CHCH}_2$ (1,3-Cyclopentadiene)	430
$\text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}=\text{CH}_2$ (1,3-Butadiene, 2-methyl-)	430
$\text{CH}_2=\text{CH}_2 + \text{cy-C}_5\text{H}_8$ (Cyclopentene)	430
$\text{CH}_2=\text{CH}_2 + \text{cy-CH}_2\text{CH}_2\text{CH}=\text{CHCH}=\text{CH}$ (1,3-Cyclohexadiene)	431
$\text{CH}_3\text{CH}_2 (+ \text{M})$	431
$\text{CH}_3\text{CH}_2 + \text{O}_2$	431
$\text{CH}_3\text{CH}_2 + \text{O}_3$	432
$\text{CH}_3\text{CH}_2 + \text{H}_2$	432
$\text{CH}_3\text{CH}_2 + \text{D}_2$	433
$\text{CH}_3\text{CH}_2 + \text{NO}$	433
$\text{CH}_3\text{CH}_2 + \text{CO}$	433
$\text{CH}_3\text{CH}_2 + \text{CH}_4$	433
$\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2$	433
$\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CHO}$	434
$\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2\text{NO}$	434
$\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CHO}$	434
$\text{CH}_3\text{CH}_2 + \text{CH}_2=\text{CHCH}_2\text{CH}_2$ (3-Butenyl)	434
$\text{CH}_3\text{CH}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2$	435
$\text{CH}_3\text{CH}_2 + \text{cy-C}_4\text{H}_7$ (Cyclobutyl)	435
$\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$	435
$\text{CH}_3\text{CH}_2 + \text{CH}_3\text{C}(\text{O})\text{C}(\text{O})\text{CH}_3$ (Biacetyl)	435
$\text{CH}_3\text{CH}_2 + (\text{CH}_3\text{CH}_2)_2\text{O}$ (Diethyl ether)	435
$\text{CH}_3\text{CH}_2 + (\text{CH}_3\text{CH}_2)_2\text{S}$ (Diethyl sulfide)	436
$\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_3$ (Diazene, diethyl-)	436
$\text{CH}_3\text{CH}_2 + (\text{CH}_3\text{CH}_2)_2\text{NOH}$ (Ethanamine, N-ethyl-N-hydroxy-)	436
$\text{CH}_3\text{CH}_2 + \text{cy-CH}_2\text{CH}_2\text{CH}=\text{CHCH}$ (2-Cyclopenten-1-yl)	436
$\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2$ (3-Pentenyl)	437
$\text{CH}_3\text{CH}_2 + \text{cy-C}_5\text{H}_9$ (Cyclopentyl)	437
$\text{CH}_3\text{CH}_2 + \text{CH}_3\text{C}(\text{O})\text{C}(\text{O})\text{CH}_2\text{CH}_3$ (2,3-Pentanedione)	437
$\text{CH}_3\text{CH}_2 + \text{cy-C}_6\text{H}_{11}$ (Cyclohexyl)	438
$\text{CH}_3\text{CH}_2 + \text{n-C}_6\text{H}_{14}$ (n-Hexane)	438
$\text{CH}_3\text{CH}_3 (+ \text{M})$	438
$\text{CH}_3\text{CH}_3^\dagger$	440

CD ₃ CD ₃	440
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C₂H_xO_y-COMPOUND Reactions:

CH=C=O + O ₂	440
CH=C=O + CH=CH	440
CH ₂ =C=O + CH ₂ =C=O	441
CH ₂ =C=O + CH ₃ COOH	441
CH ₂ =C=O + CH ₃ CH ₂ COOH	441
CH ₂ =C=O + CH ₃ CH ₂ CH ₂ COOH (Butanoic acid)	441
CH ₂ =C=O + (CH ₃) ₂ CHCOOH (Propanoic acid, 2-methyl-)	441
CH ₂ =C=O + (CH ₃) ₃ CCOOH (Propanoic acid, 2,2-dimethyl-)	441
CH ₂ =C=O + (CH ₃) ₃ CCH ₂ COOH (Butanoic acid, 3,3-dimethyl-)	441
CH ₃ CO (+ M)	441
CH ₃ CO + O ₂	442
CH ₃ CO + NO	442
CH ₃ CO + NO ₂	442
CH ₃ CO + CH ₃ CO	442
CD ₃ CO + CD ₃ CO	443
CH ₃ CO + CH ₃ CHO	443
CH ₃ CO + CH ₂ =CHCH=CH ₂	443
CH ₃ C(O)O + NO ₂	444
CH ₃ C(O)OO + NO	444
CH ₃ C(O)OO + NO ₂	444
CH ₃ C(O)OO + HCHO	444
CH ₃ C(O)OO + CH ₃ C(O)OO	445
CH ₃ C(O)OO + CH ₃ CH=CH ₂	445
CH ₃ C(O)OO + CH ₃ CH ₂ CH=CH ₂	445
CH ₃ C(O)OO + cis-CH ₃ CH=CHCH ₃	445
CH ₃ C(O)OO + trans-CH ₃ CH=CHCH ₃	445
CH ₃ C(O)OO + (CH ₃) ₂ C=CH ₂	445
CH ₃ C(O)OO + cis-CH ₃ CH=CHCH ₂ CH ₃	446
CH ₃ C(O)OO + trans-CH ₃ CH=CHCH ₂ CH ₃	446
CH ₃ C(O)OO + CH ₃ CH ₂ C(CH ₃)=CH ₂ (1-Butene, 2-methyl-)	446
CH ₃ C(O)OO + (CH ₃) ₂ CHCH=CH ₂ (1-Butene, 3-methyl-)	446
CH ₃ C(O)OO + (CH ₃) ₂ C=CHCH ₃ (2-Butene, 2-methyl-)	446
CH ₃ C(O)OO + CH ₃ CH ₂ CH ₂ CH ₂ CH=CH ₂ (1-Hexene)	446
CH ₃ CHO (+ M)	447
CH ₃ CHO + CH ₃ C(O)OOH (Ethaneperoxoic acid)	447
CH ₃ C(O)OOH + CH ₃ CH=CH ₂	447
CH ₃ C(O)OOH + CH ₃ CH ₂ CH=CH ₂	447
CH ₃ C(O)OOH + cis-CH ₃ CH=CHCH ₃	447
CH ₃ C(O)OOH + trans-CH ₃ CH=CHCH ₃	448
CH ₃ C(O)OOH + (CH ₃) ₂ C=CHCH ₃	448
CH ₃ C(O)OOH + cis-CH ₃ CH=CHCH ₂ CH ₃	448
CH ₃ C(O)OOH + trans-CH ₃ CH=CHCH ₂ CH ₃	448
CH ₃ C(O)OOH + CH ₃ CH ₂ C(CH ₃)=CH ₂ (1-Butene, 2-methyl-)	448
CH ₃ C(O)OOH + (CH ₃) ₂ CHCH=CH ₂ (1-Butene, 3-methyl-)	449
CH ₃ C(O)OOH + (CH ₃) ₂ C=CHCH ₃ (2-Butene, 2-methyl-)	449

$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ (1-Hexene)	449
$\text{CH}_3\text{CH}_2\text{O}$ (Ethoxy)	449
$\text{CH}_3\text{CH}_2\text{O} + \text{O}_2$	450
$\text{CH}_3\text{CH}_2\text{O} + \text{NO}$	450
$\text{CH}_3\text{CH}_2\text{O} + \text{NO}_2$	450
$\text{CH}_3\text{CHOH} (+ \text{M})$	450
CH_3CHOH (Ethyl, 1-hydroxy-) + O_2	450
$\text{CH}_3\text{CH}_2\text{O}_2$ (Ethyldioxy)	451
$\text{CH}_3\text{CH}_2\text{O}_2 + \text{NO}$	451
$\text{CH}_3\text{CH}_2\text{O}_2 + \text{NO}_2$	451
$\text{CH}_3\text{CH}_2\text{O}_2 + \text{CH}_2=\text{CH}_2$	452
$\text{CH}_3\text{CH}_2\text{O}_2 + \text{CH}_3\text{CH}_2\text{O}_2$	452
$\text{CH}_3\text{CH}_2\text{OH} (+ \text{M})$	452
$(\text{CH}_3)_2\text{O}$	452
CH_3OOCH_3 (Peroxide, dimethyl-)	453

$\text{C}_2\text{H}_x\text{S}_y$ -COMPOUND Reactions:

$\text{cy-CH}_2\text{CH}_2\text{S}$ (Thiirane; Ethylene episulfide)	453
$\text{cy-CH}_2\text{CH}_2\text{S}^*$ (Thiirane; Ethylene episulfide)	453
$\text{CH}_3\text{SCH}_2 + \text{CH}_4$	454

C_2N_x -COMPOUND Reactions:

$\text{NCCN} (+ \text{M})$	454
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$\text{C}_2\text{H}_x\text{N}_y$ -COMPOUND Reactions:

CH_3NC (Methane, isocyano-)	454
$(\text{CH}_3)_2\text{N} + \text{O}_2$	454
$(\text{CH}_3)_2\text{N} + \text{NO}_2$	454
$\text{CH}_3\text{N}=\text{NCH}_3$ (Azomethane; Diazene, dimethyl-)	454
$\text{CH}_3\text{N}=\text{NCH}_3^*$ (Azomethane; Diazene, dimethyl-)	455
$(\text{CH}_3)_2\text{NNH}_2$ (Hydrazine, 1,1-dimethyl-)	455
$\text{CH}_3\text{NHNHCH}_3$ (Hydrazine, 1,2-dimethyl-)	455

$\text{C}_2\text{H}_x\text{O}_y\text{N}_z$ -COMPOUND Reactions:

$\text{CH}_3\text{C}(\text{O})\text{OONO}_2$ (Peroxide, acetyl nitro-)	455
$\text{CH}_3\text{CH}_2\text{NO} + \text{CH}_3\text{CH}_2\text{NO}$ (Ethane, nitroso-)	455
$\text{CH}_3\text{CH}_2\text{NO}_2$ (Ethane, nitro-) (+ M)	455
$\text{CH}_3\text{CH}_2\text{ONO}$	456
$\text{CH}_3\text{CH}_2\text{ONO}_2$	456

C_3 (Carbon trimer) Reactions:

$\text{C}_3 + \text{O}_2$	456
$\text{C}_3 + \text{N}_2$	456
$\text{C}_3 + \text{NO}$	457

$C_3 + CH_4$	457
$C_3 + CH=CH$	457
$C_3 + CH_2=CH_2$	457
$C_3 + CH_3CH_3$	458
$C_3 + CH_3C\equiv CH$	458
$C_3 + CH_2=C=CH_2$	458
$C_3 + CH_3CH=CH_2$	458
$C_3 + CH_3CH_2CH=CH_2$	459
$C_3 + cis-CH_3CH=CHCH_3$	459
$C_3 + (CH_3)_2C=CH_2$	459
$C_3 + CH_3CH_2CH_2CH_3$	460
$C_3 + CH_3CH_2CH_2C\equiv CH$	460
$C_3 + CH_3CH=C=CHCH_3$ (2,3-Pentadiene)	460
$C_3 + (CH_3)_2C=CHCH_3$	460
$C_3 + CH_3CH_2CH_2C\equiv CCH_3$ (2-Hexyne)	460
$C_3 + (CH_3)_2C=C(CH_3)_2$	461
$C_3 + (CH_3)_2C=C=C(CH_3)_2$ (2,3-Pentadiene, 2,4-dimethyl-)	461

C_3H_x -COMPOUND Reactions:

$CH_3C\equiv CD$	461
$CH_2DC\equiv CH$	461
$CH_2=C=CH_2$ (+ M)	462
$CH_2=C=CHD$	462
cy- C_3H_4 (Cyclopropene)	462
$CH_3CH=CH^\dagger$ (1-Propenyl)	462
$CH_2=CHCH_2^\dagger$ (Allyl)	463
$CD_2=CDCD_2^\dagger$	463
$CH_2=CHCH_2 + O_2$	463
$CH_2=CHCH_2 + NO$ (+ M)	463
$CH_2=CHCH_2 + NO_2$	464
$CH_2=CHCH_2 + CH\equiv CH$	464
$CH_2=CHCH_2 + CH_2=CH_2$	464
$CH_2=CHCH_2 + CH\equiv CCH_3$	465
$CH_2=CHCH_2 + CH_2=CHCH_2$	466
$CH_3CH=CH_2$ (+ M)	466
$CH_3CH=CH_2^\dagger$	467
$CH_3CH=CH_2 + CH_3CH=CH_2$	467
$CH_3CH=CH_2 + cy-CH_2CH_2CH=CHCH=CH$ (1,3-Cyclohexadiene)	467
cy- C_3H_6 (Cyclopropane)	468
(+)-trans-cy- $CH_2CHDCHD$ (Cyclopropane-1,2- d_2 , (1S-trans)-)	469
(-)-trans-cy- $CH_2CHDCHD$ (Cyclopropane-1,2- d_2 , (1R-trans)-)	469
$CH_3CH_2CH_2$ (n-Propyl) (+ M)	470
$CH_3CH_2CH_2 + O_2$	470
$CH_3CH_2CH_2 + O_3$	471
$CH_3CH_2CH_2 + HCHO$	471
$CH_3CH_2CH_2 + CH\equiv CH$	471
$CH_3CH_2CH_2 + CH_2=CH_2$	471
$CH_3CH_2CH_2 + CH_3CH_2CH_2$	471

$\text{CH}_3\text{CH}_2\text{CH}_2 + (\text{CH}_3)_2\text{CH}$	472
$\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHO}$	472
$\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ (n-Pentyl)	472
$\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3$ (Butyl, 1-methyl-)	472
$(\text{CH}_3)_2\text{CH}$ (i-Propyl)	473
$(\text{CH}_3)_2\text{CH}^\dagger$	473
$(\text{CH}_3)_2\text{CH} + \text{O}_2$	473
$(\text{CH}_3)_2\text{CH} + \text{O}_3$	473
$(\text{CH}_3)_2\text{CH} + \text{H}_2$	474
$(\text{CH}_3)_2\text{CH} + \text{CH}_3\text{CH}_3$	474
$(\text{CH}_3)_2\text{CH} + \text{CH}_3\text{CH}=\text{CH}_2$	474
$(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CH}$	474
$(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CHCHO}$ (Propanal, 2-methyl-)	475
$(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_4\text{C}$	475
$(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$ (Butane, 2,3-dimethyl-)	475
$(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CHN}=\text{NCH}(\text{CH}_3)_2$ (Azoisopropane)	476
$\text{CH}_3\text{CH}_2\text{CH}_3 (+ \text{M})$	476
$\text{CH}_3\text{CH}_2\text{CH}_3^\dagger$	477
$\text{CD}_3\text{CD}_2\text{CD}_3$	477

$\text{C}_3\text{H}_x\text{O}_y$ -COMPOUND Reactions:

$\text{CH}_2=\text{CHCHO} + \text{cy-CH}_2\text{CH}_2\text{CH}=\text{CHCH}=\text{CH}$ (1,3-Cyclohexadiene)	477
$\text{CH}_3\text{CH}_2\text{CO} (+ \text{M})$	478
$\text{CH}_3\text{CH}_2\text{CO} + \text{O}_2$	478
$\text{CH}_2=\text{CHCH}_2\text{O}_2$ (2-Propenyldioxy)	478
$\text{CH}_3\text{CH}_2\text{CHO} + \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OOH}$ (Propaneperoxoic acid)	478
$\text{cy-CH}_2\text{CH}_2\text{CH}_2\text{O}$ (Oxetane)	478
$\text{cy-CH}(\text{CH}_3)\text{CH}_2\text{O}$ (Oxirane, methyl-)	479
$\text{HC}(\text{O})\text{OCH}_2\text{CH}_3$ (Ethyl formate)	479
$\text{CH}_3\text{C}(\text{O}^{18})\text{OCH}_3$ (Acetic- ^{18}O acid ^{16}O -methyl ester)	479
$\text{CH}_3\text{C}(\text{O})\text{OCH}_3$ (Methyl acetate)	479
$\text{CH}_3\text{CH}_2\text{CH}_2\text{O} + \text{NO}$	480
$\text{CH}_3\text{CH}_2\text{CH}_2\text{O} + \text{NO}_2$	480
$(\text{CH}_3)_2\text{CHO}$ (Ethoxy, 1-methyl-)	480
$(\text{CH}_3)_2\text{CHO} + \text{NO}$	480
$(\text{CH}_3)_2\text{CHO} + (\text{CH}_3)_2\text{CHOOH}$ (Ethoxy, 1-methyl- + Hydroperoxide, 1-methylethyl-)	481
$\text{CH}_3\text{CH}_2\text{CH}_2\text{O}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{O}_2$	481
$(\text{CH}_3)_2\text{CHO}_2$ (Ethyldioxy, 1-methyl-) + NO	481
$(\text{CH}_3)_2\text{CHO}_2 + \text{NO}_2$	481
$(\text{CH}_3)_2\text{CHO}_2 + (\text{CH}_3)_2\text{CHO}_2$	482
$(\text{CH}_3)_2\text{CHO}_2 + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$	482
$(\text{CH}_3)_2\text{CHO}_2 + (\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2$ (Ethyldioxy, 1-methyl- + Propyldioxy, 1,1,2-trimethyl-)	483
$\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$ (1-Propanol)	483
$(\text{CH}_3)_2\text{CHOH}$ (2-Propanol)	483

$C_3H_xS_y$ -COMPOUND Reactions:

cy- $CH_2CH_2CH_2S$ (Thietane; Trimethylene sulfide) 483

$C_3H_xO_yS_z$ -COMPOUND Reactions:

$CH_3C(S)OCH_3$ (Ethanethioic acid O-methyl ester) 484

cy- $CH_2CH_2CH_2S(O_2)$ (Thietane, 1,1-dioxide-;
Trimethylenesulfone) 484

$C_3H_xN_y$ -COMPOUND Reactions:

$CH_2=CHCN + NH_2CH_2CH_2CN$ (Acrylonitrile; 2-Propenenitrile) +
(β -Aminopropionitrile; Propanenitrile, 3-amino-) 484

CH_3CH_2CN (Propanenitrile) 484

cy- $CH_2CH_2CH(NH_2)$ (Cyclopropanamine) 485

$C_3H_xO_yN_z$ -COMPOUND Reactions:

$(CH_3)_2CHONO$ (Nitrous acid 1-methylethyl ester;
Isopropyl nitrite) 485

$CH_3NHC(O)OCH_3$ (Carbamic acid, methyl-, methyl ester) 486

$CH_3CH_2CH_2ONO_2$ (Nitric acid propyl ester; n-Propyl nitrate) . 486

C_4H_x -COMPOUND Reactions:

$CH=CC=C$ 486

$CH=CC=C + CH=CC=CH$ 486

$CH=CC=CH$ 486

$CH_3CH_2C=CH$ 487

$CH_3CH_2C=CH + CH_3CH_2C=CH$ 487

$CH_2=CHCH=CH_2 + CH_2=CHCH=CH_2$ 487

$CH_2=CHCH=CH_2 + cy-CH_2CH_2CH=CHCH=CH$ (1,3-Cyclohexadiene) 488

$CH_3CH_2CH=CH^\dagger$ (1-Butenyl) 488

$CH_3CH=CHCH_2 + H_2S$ 489

$CH_3CH=CHCH_2 + cis-CH_3CH=CHCH_3$ 489

trans- $CH_3CH=CHCH_2$ 489

$CH_2=CHCH_2CH_2^\dagger$ (3-Butenyl) 489

$CH_2=CHCH_2CH_2 + cy-C_4H_7$ (Cyclobutyl) 489

$CH_3C=CHCH_3^\dagger$ (1-Propenyl, 1-methyl-) 490

$CH_2=CHCHCH_3^\dagger$ (2-Propenyl, 1-methyl-) 490

trans- $CH_3CHCH=CH_2$ (2-Propenyl, 1-methyl-, (E)-) 490

$CH_2=CHCHCH_3 + CH_2=CHCHCH_3$ (1-Methylallyl) 490

$CH_2C(CH_3)=CH_2$ (2-Methylallyl) 490

$CH_2=C(CH_3)CH_2 + CH_2=C(CH_3)CH_2$ (2-Methylallyl) 491

cy- $C_4H_7 + cy-C_4H_7$ (Cyclobutyl + Cyclobutyl) 491

$CH_3CH_2CH=CH_2$ 491

cis- $CH_3CH=CHCH_3$ (+ M) 491

cis-CH ₃ CH=CHCH ₃ + H ₂ S	492
trans-CH ₃ CH=CHCH ₃ (+ M)	492
(CH ₃) ₂ C=CH ₂	492
CH ₂ CH ₂ CH ₂ CH ₂ (1,4-Butanediyl)	493
cy-C ₄ H ₈ (Cyclobutane)	493
CH ₃ CH ₂ CH ₂ CH ₂ (n-Butyl)	494
CH ₃ CH ₂ CH ₂ CH ₂ + O ₂	494
CH ₃ CH ₂ CH ₂ CH ₂ + CH ₃ CH ₂ CH ₂ CH ₂ (n-Butyl)	494
CH ₃ CH ₂ CH ₂ CH ₂ + CH ₃ CH ₂ CHCH ₃ (n-Butyl + Propyl, 1-methyl-)	495
CH ₃ CH ₂ CHCH ₃ (Propyl, 1-methyl-)	495
CH ₃ CH ₂ CHCH ₃ + O ₂	495
CH ₃ CH ₂ CHCH ₃ + CH ₃ CH ₂ CHCH ₃ (Propyl, 1-methyl- + Propyl, 1-methyl-)	496
(CH ₃) ₂ CHCH ₂ (Propyl, 2-methyl-) + O ₂	496
(CH ₃) ₃ C (t-Butyl)	496
(CH ₃) ₃ C + O ₂	497
(CH ₃) ₃ C + O ₃	497
(CH ₃) ₃ C + H ₂	498
(CH ₃) ₃ C + NO	498
(CH ₃) ₃ C + (CH ₃) ₃ C	498
CH ₃ CH ₂ CH ₂ CH ₃	499
(CH ₃) ₃ CH (Isobutane)	499
(CH ₃) ₃ CH [†] (Isobutane)	500

C₄H_xO_y-COMPOUND Reactions:

CH≡CCH ₂ COOH (3-Butynoic acid)	500
CH≡CCH ₂ COOD (3-Butynoic acid-d)	500
CH ₂ C(O)C(O)CH ₃ (Butyl, 2,3-dioxo-)	501
cy-CH ₂ CH ₂ CH ₂ C(O) (Cyclobutanone)	501
(+)-(S)-cy-CH(CH=CH ₂)CH ₂ O (Oxirane, ethenyl-, (S)-)	501
(S)-cis-cy-CH(CH=CH ₂)CHDO (Oxirane-d, 3-ethenyl-, cis-, (S)-)	502
trans-cy-CH(CH=CH ₂)CHDO (Oxirane-d, 3-ethenyl, trans-)	502
cy-CH(CH=CH ₂)CD ₂ O (Oxirane-2,2-d ₂ , ethenyl-)	503
CH ₂ =CHCH ₂ COOH (3-Butenoic acid)	503
CH ₃ C(O)C(O)CH ₃ (2,3-Butanedione)	503
CH ₃ CH ₂ CH ₂ CO (Butyl, 1-oxo-)	503
CH ₂ CH ₂ C(O)CH ₃ (Butyl, 3-oxo-)	503
CH ₃ CH ₂ CHCHO (Propyl, 1-formyl-)	504
(CH ₃) ₂ CCHO (Ethyl, 1,1-dimethyl-2-oxo-) (+ M)	504
CH ₃ CH(OH)CH=CH ₂ (3-Buten-2-ol)	504
CH ₃ OCH ₂ CH=CH ₂ (1-Propene, 3-methoxy-)	504
CH ₃ CH ₂ OCH=CH ₂ (Ethene, ethoxy-)	504
CH ₃ CH ₂ C(O)CH ₃ (+ M)	504
cy-CH(CH ₂ CH ₃)CH ₂ O (Oxirane, ethyl-)	505
cy-C(CH ₃) ₂ CH ₂ O (Oxirane, 2,2-dimethyl-)	505
cis-cy-CH(CH ₃)CH(CH ₃)O (Oxirane, 2,3-dimethyl-, cis-; cis-2,3-Epoxybutane)	506

trans-cy-CH(CH ₃)CH(CH ₃)O (Oxirane, 2,3-dimethyl-, trans-; trans-2,3-Epoxybutane)	506
cy-CH ₂ CH ₂ CH(CH ₃)O (Oxetane, 2-methyl-)	507
CH ₃ C(O)OCH ₂ CH ₃ (Ethyl acetate)	507
CH ₃ OC(O)OCH ₂ CH ₃ (Carbonic acid ethyl methyl ester)	508
CH ₃ CH(OH)CHCH ₃ (Propyl, 2-hydroxy-1-methyl-) + O ₂	508
CH ₃ CH ₂ CH ₂ CH ₂ O (Butoxy)	508
CH ₃ CH ₂ CH(O·)CH ₃ (Propoxy, 1-methyl-)	508
CH ₃ CH ₂ CH(O·)CH ₃ + NO	508
CH ₃ CH ₂ CH(O·)CH ₃ + NO ₂	509
(CH ₃) ₃ CO (t-Butoxy)	509
(CH ₃) ₃ CO + NO	509
(CH ₃) ₃ CO + HCHO	510
(CH ₃) ₃ CO + CH ₃ CHO	510
(CH ₃) ₃ CO + CD ₃ CHO	510
(CH ₃) ₃ CO + (CH ₃) ₂ CO	511
(CH ₃) ₃ CO + (CD ₃) ₂ CO	511
(CH ₃) ₃ CO + (CH ₃) ₃ CH	511
(CH ₃) ₃ CO ₂ + NO	511
(CH ₃) ₃ CO ₂ + NO ₂	512
(CH ₃) ₃ CO ₂ + (CH ₃) ₃ CO ₂	512
(CH ₃) ₂ CCH ₂ OOH (Ethyl, 1-(hydroperoxymethyl)-1-methyl-)	512
(CH ₃) ₂ CHCH ₂ O ₂ (Propyldioxy, 2-methyl-)	513
(CH ₃) ₂ C(OO·)CH ₂ OOH (Ethyldioxy, 1-(hydroperoxymethyl)-1-methyl)	513
(CH ₃) ₃ COH (t-Butanol)	513
(CH ₃ CH ₂) ₂ O (Diethyl ether)	513

C₄H_xS_y-COMPOUND Reactions:

CH ₃ SCH ₂ CH=CH ₂ (1-Propene, 3-(methylthio)-)	514
CH ₃ C(S)SCH ₂ CH ₃ (Ethane(dithioic) acid ethyl ester)	514

C₄H_xO_yS_z-COMPOUND Reactions:

CH ₃ C(O)SCH ₂ CH ₃ (Ethanethioic acid S-ethyl ester)	514
CH ₃ C(S)OCH ₂ CH ₃ (Ethanethioic acid O-ethyl ester)	514
CH ₃ OC(S)OCH ₂ CH ₃ (Carbonothioic acid O-ethyl O-methyl ester)	515
CH ₃ OC(O)SCH ₂ CH ₃ (Carbonothioic acid S-ethyl O-methyl ester)	515
CH ₃ CH ₂ OC(O)SCH ₃ (Carbonothioic acid O-ethyl S-methyl ester)	515
CH ₃ SC(S)OCH ₂ CH ₃ (Carbonodithioic acid O-ethyl S-methyl ester)	515

C₄H_xN_y-COMPOUND Reactions:

CH ₂ =CHCH ₂ NC (1-Propene, 3-isocyano-)	515
cis-CH ₃ CH=CHCN (cis-Crotononitrile)	516
cy-CH ₂ CH ₂ CH(CN) (Cyclopropanecarbonitrile; Cyclopropyl cyanide)	516
CH ₃ CH ₂ CH ₂ CN (Butanenitrile)	516

$(\text{CH}_3)_2\text{CHCN}$ (Propanenitrile, 2-methyl-)	516
$\text{CH}_2=\text{CHCH}_2\text{NHCH}_3$ (2-Propen-1-amine, N-methyl-)	517
$\text{CH}_3\text{N}=\text{NCH}_2\text{CH}=\text{CH}_2$ (Diazene, methyl-(2-propenyl)-)	517
$\text{CH}_3\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_3$ (Azoethane)	517
$\text{CH}_3\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_3^*$ (Azoethane)	517
$(\text{CH}_3)_2\text{NN}(\text{CH}_3)_2$ (Hydrazine, tetramethyl-)	517

$\text{C}_4\text{H}_x\text{O}_y\text{N}_z$ -COMPOUND Reactions:

$\text{NCC}(\text{O})\text{OCH}_2\text{CH}_3$ (Ethyl cyanofornate)	518
$(\text{CH}_3)_3\text{CNO}$	518
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{ONO}$ (n-Butyl nitrite)	518
$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{ONO}$ (s-Butyl nitrite)	518
$(\text{CH}_3)_3\text{CONO}$ (t-Butyl nitrite)	518
$(\text{CH}_3)_3\text{CONO}_2$ (t-Butyl nitrate)	519
$(\text{CH}_3\text{CH}_2)_2\text{NO}$ (Nitroxide, diethyl-) + NO_2	519
$(\text{CH}_3\text{CH}_2)_2\text{NOH}$ (Ethanamine, N-ethyl-N-hydroxy-) + NO_2	519
$(\text{CH}_3\text{CH}_2\text{NO})_2$ (Nitrosoethane dimer; Diazene, diethyl-, 1,2-dioxide)	519

C_5H_x -COMPOUND Reactions:

$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}\equiv\text{CH}$ (1-Pentyne)	520
$\text{CH}_3\text{CH}_2\text{C}\equiv\text{CCH}_3$ (2-Pentyne)	520
$(\text{CH}_3)_2\text{CHC}\equiv\text{CH}$ (1-Butyne, 3-methyl-)	520
cis- $\text{CH}_3\text{CH}=\text{CHCH}=\text{CH}_2$ (cis-1,3-Pentadiene)	520
cis- $\text{CH}_3\text{CH}=\text{CHCH}=\text{CH}_2^\dagger$ (cis-1,3-Pentadiene)	521
trans- $\text{CH}_3\text{CH}=\text{CHCH}=\text{CH}_2$ (trans-1,3-Pentadiene)	521
$(\text{CH}_3)_2\text{C}=\text{C}=\text{CH}_2$ (1,2-Butadiene, 3-methyl-)	521
cy- C_5H_8 (Cyclopentene)	521
cy- $\text{CH}(\text{CH}=\text{CH}_2)\text{CH}_2\text{CH}_2\text{O}$ (Cyclopropane, ethenyl-)	522
$(\text{CH}_2)_2>\text{C}<(\text{CH}_2)_2$ (Spiropentane)	522
$[\text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_3 = \text{CH}_2=\text{CHCHCH}_2\text{CH}_3]$ (2-Pentenyl = 2-Propenyl, 1-ethyl-)	523
$[\text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_3 = \text{CH}_2=\text{CHCHCH}_2\text{CH}_3]$ (2-Pentenyl = 2-Propenyl, 1-ethyl-) + O_2	523
$\text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_3$ (2-Pentenyl) + CH_3CHO	523
$\text{CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2$ (3-Pentenyl)	523
$\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2^\dagger$ (4-Pentenyl)	524
$\text{CH}_3\text{CHCH}_2\text{CH}=\text{CH}_2^\dagger$ (3-Butenyl, 1-methyl-)	524
$\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2^\dagger$ (3-Butenyl, 2-methyl-)	524
cy- C_5H_9 + cy- C_5H_9 (Cyclopentyl + Cyclopentyl)	524
cy- C_5D_9 + cy- C_5D_9 (Cyclopentyl-d ₉ + Cyclopentyl-d ₉)	525
cy- C_5H_9 + cy- C_6H_{11} (Cyclopentyl + Cyclohexyl)	525
cy- C_5H_9 + cy- C_6D_{11} (Cyclopentyl + Cyclohexyl-d ₁₁)	526
cy- C_5D_9 + cy- C_6H_{11} (Cyclopentyl-d ₉ + Cyclohexyl)	526
cy- C_5D_9 + cy- C_6D_{11} (Cyclopentyl-d ₉ + Cyclohexyl-d ₁₁)	527
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ (1-Pentene)	527
$\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3$ (2-Pentene, cis-trans mixture)	528

cis-CH ₃ CH ₂ CH=CHCH ₃ (cis-2-Pentene) (+ M)	528
trans-CH ₃ CH ₂ CH=CHCH ₃ (trans-2-Pentene) (+ M)	528
CH ₃ CH ₂ C(CH ₃)=CH ₂ (1-Butene, 2-methyl-)	528
CH ₃ CH ₂ C(CH ₃)=CH ₂ [†] (1-Butene, 2-methyl-)	528
(CH ₃) ₂ CHCH=CH ₂ [†] (1-Butene, 3-methyl-)	529
cy-C ₅ H ₁₀ (Cyclopentane)	529
cis-cy-CH(CH ₃)CH(CH ₃)CH ₂ (Cyclopropane, 1,2-dimethyl-, cis-)	530
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ (Pentyl)	530
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ [†] (Pentyl)	530
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ (Pentyl) + O ₂	530
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ + CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ (Pentyl + Pentyl)	531
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ + CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ N=NCH ₃ (Diazene, methylpentyl-)	531
CH ₃ CH ₂ CH ₂ CHCH ₃ (Butyl, 1-methyl-)	531
CH ₃ CH ₂ CH ₂ CHCH ₃ [†] (Butyl, 1-methyl-)	531
CD ₃ CD ₂ CD ₂ CD ₃ [†] (Butyl-1,2,2,3,3,4,4,4-d ₈ , 1-methyl-d ₃)	531
CH ₃ CH ₂ CH ₂ CHCH ₃ (Butyl, 1-methyl-) + O ₂	532
CH ₃ CH ₂ CH ₂ CHCH ₃ + CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ (Butyl, 1-methyl- + Pentyl)	532
CH ₃ CH ₂ CHCH ₂ CH ₃ (Propyl, 1-ethyl-)	532
CH ₃ CH ₂ CHCH ₂ CH ₃ (Propyl, 1-ethyl-) + O ₂	532
(CH ₃) ₃ CCH ₂ (Propyl, 2,2-dimethyl-) (+ M)	532
CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ (n-Pentane)	533
CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ [†] (n-Pentane)	533
(CH ₃) ₂ CHCH ₂ CH ₃ [†] (Isopentane)	533
(CH ₃) ₄ C (Neopentane)	534

C₅H_xO_y-COMPOUND Reactions:

CH ₃ C≡CCH ₂ COOH (3-Pentynoic acid)	534
CH ₃ C≡CCH ₂ COOD (3-Pentynoic acid-d)	534
CH ₂ =C=CHCH ₂ COOH (3,4-Pentadienoic acid)	534
cy-CH ₂ CH ₂ CH=C(CH ₃)O (Furan, 2,3-dihydro-5-methyl-)	535
(cy-CH ₂ CH ₂ CH)C(O)CH ₃ (Ethanone, 1-cyclopropyl-)	535
bicy-C ₅ H ₈ O (6-Oxabicyclo[3.1.0]hexane)	535
CH ₃ CH=CHCH ₂ COOH (3-Pentenoic acid)	536
CH ₃ C(O)C(O)CH ₂ CH ₃ (2,3-Pentanedione)	536
CH ₂ =C(CH ₃)CH ₂ COOH (3-Butenoic acid, 3-methyl-)	536
(cy-CH ₂ CH ₂ CH)CH ₂ COOH (Cyclopropaneacetic acid)	536
CH ₃ CH ₂ OCH ₂ CH=CH ₂ (1-Propene, 3-ethoxy-)	537
CH ₃ CH ₂ CH ₂ OCH=CH ₂ (Propane, 1-(ethenyloxy)-)	537
cy-CH ₂ CH ₂ CH(CH ₂ CH ₃)O (Oxetane, 2-ethyl-)	537
cy-CH ₂ CH ₂ C(CH ₃) ₂ O (Oxetane, 2,2-dimethyl-)	537
cis-cy-CH ₂ CH(CH ₃)CH(CH ₃)O (Oxetane, 2,3-dimethyl-, cis-)	538
trans-cy-CH ₂ CH(CH ₃)CH(CH ₃)O (Oxetane, 2,3-dimethyl-, trans-)	538
cy-CH(CH ₃)C(CH ₃) ₂ O (Oxirane, trimethyl-)	538
CH ₃ OCH ₂ CH ₂ OCH=CH ₂ (Ethene, (2-methoxyethoxy)-)	539
CH ₃ C(O)OCH ₂ CH ₂ CH ₃ (n-Propyl acetate)	539
CH ₃ C(O)OCH(CH ₃) ₂ (i-Propyl acetate)	539
CH ₃ CH ₂ C(O)OCH ₂ CH ₃ (Propanoic acid ethyl ester)	539

CH ₃ CH ₂ OC(O)OCH ₂ CH ₃	(Carbonic acid diethyl ester)	540
CH ₃ C(O)OCH ₂ CH ₂ OCH ₃	(Ethanol, 2-(methoxy)-, acetate)	540
HOCH ₂ C(O)OCH(CH ₃) ₂	(Acetic acid, hydroxy-, 1-methylethyl ester)	540
CH ₃ CH ₂ C(CH ₃) ₂ O	(Propoxy, 1,1-dimethyl-)	540
CH ₃ CH ₂ C(CH ₃) ₂ O	(Propoxy, 1,1-dimethyl-) + NO	540
(CH ₃) ₃ CCH ₂ OO	(Propyldioxy, 2,2-dimethyl-)	541
CH ₃ CH(OOH)CH ₂ CHCH ₃	(Butyl, 3-hydroperoxy-1-methyl-)	541
HOCH ₂ CH ₂ CHCH ₂ CH ₃	(Propyl, 3-hydroperoxy-1-ethyl-)	541
(CH ₃) ₂ C(CH ₂ OOH)CH ₂	(Propyl, 2-methyl-2-hydroperoxymethyl-)	541
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ OO	(Pentyldioxy)	541
CH ₃ CH ₂ CH ₂ CH(O ₂)CH ₃	(Butyldioxy, 1-methyl-)	542
CH ₃ CH(OOH)CH ₂ CH(OO·)CH ₃	(Butyldioxy, 3-hydroperoxy-1-methyl-)	542
CH ₃ CH ₂ CH(OO)CH ₂ CH ₂ OOH	(Propyldioxy, 3-hydroperoxy-1-ethyl-)	542
(CH ₃) ₂ C(CH ₂ OOH)CH ₂ OO	(Propyldioxy, 2-hydroperoxymethyl-2-methyl-)	542
(CH ₃) ₃ COCH ₃	(Propane, 2-methoxy-2-methyl-)	542

C₅H_xO_yS_z-COMPOUND Reactions:

CH ₃ C(O)SCH(CH ₃) ₂	(Ethanethioic acid S-(1-methylethyl) ester)	543
CH ₃ C(S)OCH(CH ₃) ₂	(Ethanethioic acid O-(1-methylethyl) ester)	543
CH ₃ C(O)OCH ₂ CH ₂ SCH ₃	(Ethanol, 2-(methylthio)-, acetate)	543
CH ₃ C(O)SCH(CH ₃)OCH ₃	(Ethanethioic acid S-(1-methoxyethyl ester)	543
CH ₃ OC(S)OCH(CH ₃) ₂	(Carbonothioic acid O-methyl O-(1-methylethyl) ester)	543
CH ₃ OC(O)SCH(CH ₃) ₂	(Carbonothioic acid O-methyl S-(1-methylethyl) ester)	544
(CH ₃) ₂ CHOC(O)SCH ₃	(Carbonothioic acid S-methyl O-(1-methylethyl) ester)	544
cy-CH ₂ CH(CH ₃)CH ₂ CH ₂ S(O ₂)	(Thiophene, tetrahydro-3-methyl- 1,1-dioxide; 3-Methylsulfolane)	544
CH ₃ SC(S)OCH(CH ₃) ₂	(Carbonodithioic acid S-methyl O-(1-methylethyl) ester)	544
CH ₃ OC(S)SCH(CH ₃) ₂	(Carbonodithioic acid O-methyl S-(1-methylethyl) ester)	544

C₅H_xN_y-COMPOUND Reactions:

cy-CH ₂ CH ₂ CH=CHC(CN)	(1-Cyclobutene-1-carbonitrile)	545
bicy-C ₄ H ₅ (CN)	(Bicyclo[1.1.0]butane-1-carbonitrile)	545
cy-CH ₂ CH ₂ CH ₂ C(CN)	(Cyclobutanecarbonitrile)	545
(CH ₃) ₂ CHCH ₂ CN	(Butanenitrile, 3-methyl-)	546
(CH ₃) ₃ CCN	(Propanenitrile, 2,2-dimethyl-)	546
CH ₃ CH ₂ N=NCH(CH ₃) ₂	(Diazene, ethyl-(1-methylethyl)-)	546
CH ₃ CH ₂ C(CH ₃) ₂ NH ₂	(2-Butanamine, 2-methyl-, or t-Amylamine)	546

$C_5H_xO_yN_z$ -COMPOUND Reactions:

$CH_3C(O)OCH_2CH_2CN$ (Propanenitrile, 3-(acetyloxy)-)	547
$CH_3CH_2C(CH_3)_2ONO$ (1,1-Dimethylpropyl nitrite)	547
$(CH_3)_2NC(O)OCH_2CH_3$ (Carbamic acid, dimethyl-, ethyl ester)	547

C_6H_x -COMPOUND Reactions:

trans- $CH_2=CHCH=CHCH=CH_2$ (1,3,5-Hexatriene, (E)-)	547
cis- $CH_3CH=C=CHCH_3$ (2,3,4-Hexatriene, (Z)-)	547
cy- $CH_2CH_2CH=CHCH=CH$ (1,3-Cyclohexadiene)	547
cy- $CH_2CH_2CH=CHCH=CH$ + cy- $CH_2CH_2CH=CHCH=CH$ (1,3-Cyclohexadiene + 1,3-Cyclohexadiene)	548
$CH=CCH_2CH_2CH_2CH_3$ (1-Hexyne)	550
$CH_3C\equiv CCH(CH_3)_2$ (2-Pentyne, 4-methyl-)	550
$(CH_3)_3CC\equiv CH$ (1-Butyne, 3,3-dimethyl-)	550
$CH_3CH_2CH=CHCH=CH_2$ (1,3-Hexadiene)	551
$CH_2=CHCH_2CH_2CH=CH_2$ (1,5-Hexadiene)	551
$CH_2=CHCH_2CH_2CH=CD_2$ (1,5-Hexadiene-1,1-d ₂)	551
cis- $CH_3CH=C(CH_3)CH=CH_2$ (1,3-Pentadiene, 3-methyl-, (Z)-)	551
$CH_2=CHCH(CH_3)CH=CH_2$ (1,4-Pentadiene, 3-methyl-)	551
cy- C_6H_{10} (Cyclohexene)	551
cy- $CH_2CH_2CH_2C(=CHCH_3)$ (Cyclobutane, ethylidene-)	552
cy- $CH_2CH_2C(=CH_2)CH(CH_3)$ (Cyclobutane, 1-methyl-2-methylene-)	552
cy- $CH(CH_3)CH_2C(=CH_2)CH_2$ (Cyclobutane, 1-methyl-3-methylene-)	552
Spiro- $[CH(CH_3)CH_2]>C<(CH_3)_2$ (Spiropentane, methyl-)	553
$CH_2CH_2CH_2CH_2CH=CH_2^\dagger$ (5-Hexenyl)	553
cy- $(CH_2)_5CH$ + cy- $(CH_2)_5CH$ (Cyclohexyl + Cyclohexyl)	554
cy- $(CD_2)_5CD$ + cy- $(CD_2)_5CD$ (Cyclohexyl-d ₁₁ + Cyclohexyl-d ₁₁)	554
cy- $(CH_2)_5CH$ + (cy- C_6H_{11}) $N=N(C_6H_{11}$ -cy) (Cyclohexyl + Azocyclohexane)	555
$CH_2=CH(CH_2)_3CH_3$ (1-Hexene)	555
cis- $CH_3CH_2CH_2CH=CHCH_3$ (2-Hexene, (Z)-)	555
$(CH_3)_2CHC(CH_3)=CH_2$ (1-Butene, 2,3-dimethyl-)	555
$(CH_3)_3CCH=CH_2$ (1-Butene, 3,3-dimethyl-)	556
cis- $CH(CH_3)CH(CH_3)CH_2CH_2$ (1,4-Butanediyl, 1,2-dimethyl- (Z)-)	556
trans- $CH(CH_3)CH(CH_3)CH_2CH_2$ (1,4-Butanediyl, 1,2-dimethyl-, (E)-)	556
cy- C_6H_{12} (Cyclohexane)	557
trans-cy- $CH_2CH_2CH(CH_3)CH(CH_3)$ (Cyclobutane, 1,2-dimethyl-, trans-)	558
cy- $C(CH_3)_2CH(CH_3)CH_2$ (Cyclopropane, 1,1,2-trimethyl-)	559
$CH_3CHCH_2CH_2CH_2CH_3^\dagger$ (Pentyl, 1-methyl-)	560
$(CH_3)_2CHCH(CH_3)CH_2$ (Butyl, 2,3-dimethyl-)	560
n- C_6H_{14} (n-Hexane)	560
$(CH_3)_2CHCH_2CH_2CH_3$ (Pentane, 2-methyl-)	561
$(CH_3)_3CCH_2CH_3$ (Butane, 2,2-dimethyl-)	561
$(CH_3)_3CCH_2CH_3^\dagger$ (Butane, 2,2-dimethyl-)	561

$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$ (Butane, 2,3-dimethyl-)	561
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$\text{C}_6\text{H}_x\text{O}_y$ -COMPOUND Reactions:

$\text{CH}=\text{CC}(\text{CH}_3)_2\text{COOH}$ (3-Butynoic acid, 2,2-dimethyl-)	562
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{C}=\text{CH}$ (3-Butyn-1-ol acetate)	562
$(\text{CH}_2=\text{CHCH}_2)_2\text{O}$ (Diallylether)	562
bicy- $\text{C}_6\text{H}_{10}\text{O}$ (1,2-Epoxy cyclohexane)	562
bicy- $\text{C}_6\text{H}_6\text{D}_4\text{O}$ (7-Oxabicyclo[4.1.0]heptane-2,2,5,5- d_4)	563
$\text{CH}_2=\text{CHC}(\text{CH}_3)_2\text{COOH}$ (3-Butenoic acid, 2,2-dimethyl-)	563
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}=\text{CH}_2$ (3-Buten-1-ol acetate)	563
[cy- $\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)$] CH_2COOH (Cyclopropaneacetic acid, 1-methyl-)	563
trans-[cy- $\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}$] CH_2COOH (Cyclopropaneacetic acid, 2-methyl-, trans-)	564
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3$ (2-Butanone, 4-(acetyloxy)-)	564
$(\text{CH}_3)_2\text{CHCH}_2\text{OCH}=\text{CH}_2$ (Propane, 1-(ethenyloxy)-2-methyl-)	564
$(\text{CH}_3)_2\text{CHOC}(\text{CH}_3)=\text{CH}_2$ (1-Propene, 2-(1-methylethoxy)-)	564
$(\text{CH}_3)_3\text{COCH}=\text{CH}_2$ (Propane, 2-(ethenyloxy)-2-methyl-)	565
cy- $(\text{CH}_3)\text{C}(\text{CH}_2\text{CH}_3)\text{CH}_2\text{OCH}_2$ (Oxetane, 3-ethyl-3-methyl-)	565
cy- $\text{C}(\text{CH}_3)_2\text{C}(\text{CH}_3)_2\text{O}$ (Oxirane, tetramethyl-)	565
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (n-Butyl acetate)	565
$\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$ (Propanoic acid 1-methylethyl ester)	565
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_3$ (t-Butyl acetate)	566
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CD}_3)_3$ (t-Butyl-d ₉ acetate)	566
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{OCH}_3$ (1-Propanol, 3-methoxy-, acetate)	566
$\text{CH}_3\text{OCH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$ (Acetic acid, methoxy-, 1-methylethyl ester)	566
$\text{CH}_3\text{CH}_2\text{OC}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_3$ (Carbonic acid ethyl propyl ester)	566
$(\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2$ (Propoxy, 1,1,2-trimethyl-)	566
$(\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2$ (Propoxy, 1,1,2-trimethyl-) + O_2	566
$(\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$	567
$(\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2$ (Propyldioxy, 1,1,2-trimethyl-) + $(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$	567
$(\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2 + (\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2$	567
$(\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2$ (Propyldioxy, 1,1,2-trimethyl-)	567
$(\text{CH}_3)_2\text{CHC}(\text{CH}_3)_2\text{OH}$ (2-Butanol, 2,3-dimethyl-)	567
$(\text{CH}_3)_3\text{CCH}(\text{CH}_3)\text{OH}$ (2-Butanol, 3,3-dimethyl-)	568

$\text{C}_6\text{H}_x\text{S}_y$ -COMPOUND Reactions:

$\text{CH}_2=\text{CHCH}_2\text{SCH}_2\text{CH}=\text{CH}_2$ (Diallyl sulfide)	568
$\text{CH}_3\text{CH}_2\text{CH}_2\text{SCH}_2\text{CH}=\text{CH}_2$ (1-Propene, 3-(propenylthio)-)	568

$\text{C}_6\text{H}_x\text{O}_y\text{S}_z$ -COMPOUND Reactions:

$\text{CH}_3\text{C}(\text{S})\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (Ethanethioic acid O-butyl ester)	568
$\text{CH}_3\text{C}(\text{S})\text{OCH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ (Ethanethioic acid O-(1-methylpropyl) ester)	569

CH ₃ C(S)OCH ₂ CH(CH ₃) ₂	(Ethanethioic acid O-(2-methylpropyl) ester)	 569
CH ₃ C(O)SCH ₂ CH ₂ CH ₂ CH ₃	(Ethanethioic acid S-butyl ester)	 569
CH ₃ C(O)SCH ₂ CH(CH ₃) ₂	(Ethanethioic acid S-(2-methylpropyl) ester)	 569
CH ₃ C(O)SCH(CH ₃)CH ₂ CH ₃	(Ethanethioic acid S-(1-methylpropyl) ester)	 570
CH ₃ C(O)SC(CH ₃) ₃	(Ethanethioic acid S-(1,1-dimethylethyl) ester)	 570
CH ₃ OC(O)SC(CH ₃) ₃	(Carbonothioic acid S-(1,1-dimethylethyl) ester)	 570
(CH ₃) ₃ COC(O)SCH ₃	(Carbonothioic acid O-(1,1-dimethylethyl) ester)	 570
CH ₃ C(S)SCH ₂ CH ₂ CH ₂ CH ₃	(Ethane(dithioic) acid butyl ester)	 570
CH ₃ C(S)SCH(CH ₃)CH ₂ CH ₃	(Ethane(dithioic) acid 1-methylpropyl ester)	 571
CH ₃ C(S)SC(CH ₃) ₃	(Ethane(dithioic) acid 1,1-dimethylethyl ester)	 571
CH ₃ OC(S)SC(CH ₃) ₃	(Carbonodithioic acid S-(1,1-dimethylethyl) ester)	 571

C₆H_xN_y-COMPOUND Reactions:

trans-cy-CH ₂ CH ₂ CH(CN)CH(CN)	(1,2-Cyclobutanedicarbonitrile, trans-)	 571
cy-CH ₂ C(=CH ₂)CH ₂ CH(CN)	(Cyclobutanecarbonitrile, 3-methylene-)	 571
(cy-CH ₂ CH ₂ CH)N=CHCH ₂ CH ₃	(Cyclopropanamine, N-propylidene-)	.. 572
cy-CH(CH ₂ CH ₃)CH ₂ CH ₂ CH=N	(2H-Pyrrole, 2-ethyl-3,4-dihydro-)	.. 572
CH ₂ =CHCH ₂ NHCH ₂ CH=CH ₂	(2-Propen-1-amine, N-(2-propenyl)-)	 572
(CH ₃) ₂ CHN=NCH ₂ CH=CH ₂	(Diazene, (1-methylethyl)-2-propenyl-)	. 572
CH ₃ CH ₂ CH ₂ N=NCH ₂ CH ₂ CH ₃ [*]	(Azo-n-propane)	 573
(CH ₃) ₂ CHN=NCH(CH ₃) ₂	(Azoisopropane)	 573
(CH ₃) ₂ CHN=NCH(CH ₃) ₂ [*]	(Azoisopropane)	 573

C₆H_xO_yN_z-COMPOUND Reactions:

CH ₃ CONHC(CH ₃) ₃	(Acetamide, N-(1,1-dimethylethyl)-) (+ M)	 574
CH ₃ C(O)OC(CH ₃) ₂ CN	(Propanenitrile, 2-(acetyloxy)-2-methyl-)	. 574
CH ₃ C(O)OCH ₂ CH ₂ N(CH ₃) ₂	(Acetic acid 2-(dimethylamino)ethyl ester)	 574
(CH ₃) ₂ NC(O)OCH(CH ₃) ₂	(Carbamic acid, dimethyl-, 1-methylethyl ester)	 574

C₇H_x-COMPOUND Reactions:

CH≡CCH ₂ CH ₂ CH ₂ C≡CH	(1,6-Heptadiyne)	 574
CH ₂ =C=CHCH(CH ₃)C≡CH	(1,2-Hexadien-5-yne, 4-methyl-)	 574
cy-CH=CHCH=CHCH=CHCH ₂	(1,3,5-Cycloheptatriene)	 575

bicy-C ₇ H ₈ (Bicyclo[2.2.1]hepta-2,5-diene; 2,5-Norbornadiene)	575
bicy-C ₇ H ₁₀ (Bicyclo[2.2.1]hept-2-ene; Norbornene)	575
bicy-C ₇ H ₁₀ (Bicyclo[3.2.0]hept-2-ene)	576
tricy-C ₆ H ₁₀ (Tricyclo[4.1.1.0 ^{1,3}]heptane)	576
CH≡CCH ₂ CH(CH ₃)CH ₂ CH ₃ (1-Hexyne, 4-methyl-)	577
CH≡CCH ₂ CH ₂ CH(CH ₃) ₂ (1-Hexyne, 5-methyl-)	577
CH ₃ C≡CC(CH ₃) ₃ (2-Pentyne, 4,4-dimethyl-)	577
CH ₂ =CHCH ₂ CH ₂ CH ₂ CH=CH ₂ (1,6-Heptadiene)	578
cis-CH ₂ =C(CH ₃)C(CH ₃)=CHCH ₃ (1,3-Pentadiene, 2,3-dimethyl-, (Z)-)	578
trans-CH ₂ =C(CH ₃)C(CH ₃)=CHCH ₃ (1,3-Pentadiene, 2,3-dimethyl-, (E)-)	578
CH ₂ =CHC(CH ₃)=C(CH ₃) ₂ (1,3-Pentadiene, 3,4-dimethyl-)	578
cy-(CH ₂) ₄ CH=C(CH ₃) (Cyclohexene, 1-methyl-)	579
(-)-C(CH ₂ CH ₃)=CHCH(CH ₂ CH ₃) (Cyclopropene, 1,3-diethyl-, (-)-)	579
(+)-C(CH ₂ CH ₃)=CHCH(CH ₂ CH ₃) (Cyclopropene, 1,3-diethyl-, (+)-)	580
bicy-C ₇ H ₁₂ (Bicyclo[4.1.0]heptane)	580
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH=CH ₂ (1-Heptene)	581
cis-CH ₃ CH ₂ CH ₂ CH ₂ CH=CHCH ₃ (2-Heptene, (Z)-)	581
(CH ₃) ₂ CHCH=C(CH ₃) ₂ (2-Pentene, 2,4-dimethyl-)	581
cy-C(CH ₃) ₂ CH(CH ₃)CH ₂ CH ₂ (Cyclobutane, 1,1,2-trimethyl-)	581
cy-C(CH ₃) ₂ C(CH ₃) ₂ CH ₂ (Cyclopropane, 1,1,2,2-tetramethyl-)	582
(CH ₃) ₂ CHCH ₂ C(CH ₃) ₂ [†] (Butyl, 1,1,3-trimethyl-)	582
(CH ₃) ₃ CCH ₂ CHCH ₃ [†] (Butyl, 1,3,3-trimethyl-)	582
(CH ₃) ₂ CHC(CH ₃) ₂ CH ₂ (Butyl, 2,2,3-trimethyl-)	582
(CH ₃) ₃ CCH(CH ₃)CH ₂ (Butyl, 2,3,3-trimethyl-)	582
(CH ₃) ₃ CC(CH ₃) ₂ (Propyl, 1,1,2,2-tetramethyl-)	583
(CH ₃) ₃ CC(CH ₃) ₂ + O ₂	583
n-C ₇ H ₁₆ (n-Heptane)	584
(CH ₃) ₂ CHCH ₂ CH(CH ₃) ₂ (Pentane, 2,4-dimethyl-)	584
(CH ₃) ₃ CCH(CH ₃) ₂ (Butane, 2,2,3-trimethyl-)	584

C₇H_xO_y-COMPOUND Reactions:

bicy-C ₇ H ₈ O (Bicyclo[3.2.0]hept-2-en-6-one)	584
bicy-C ₇ H ₁₀ O (Bicyclo[3.2.0]heptan-6-one)	584
CH ₂ =C=CHC(CH ₃) ₂ COOH (3,4-Pentadienoic acid, 2,2-dimethyl-)	584
CH ₂ =C(CH ₃)C(CH ₃) ₂ COOH (3-Butenoic acid, 2,2,3-trimethyl-)	585
CH ₃ C(O)OCH ₂ CH ₂ CH ₂ CH=CH ₂ (4-Penten-1-ol acetate)	585
CH ₃ C(O)OCH(CH ₃)CH ₂ CH=CH ₂ (4-Penten-2-ol acetate)	585
trans-CH ₃ CH=CHCOOCH(CH ₃) ₂ (2-Butenoic acid, (E)-, 1-methylethyl ester)	585
[cy-(CH ₂) ₅ CH]OC(O)H (Cyclohexyl formate)	585
[cy-(CH ₂) ₄ CH]OC(O)CH ₃ (Cyclopentanol acetate)	585
(cy-CH ₂ CH ₂ CH)C(CH ₃) ₂ COOH (Cyclopropaneacetic acid, α,α-dimethyl-)	586
[cy-CH ₂ C(CH ₃) ₂ CH]CH ₂ COOH (Cyclopropaneacetic acid, 2,2-dimethyl-)	586
CH ₃ C(O)OCH ₂ CH ₂ CH ₂ COCH ₃ (2-Pentanone, 5-acetyloxy-)	586

$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{COCH}_3$	(2-Butanone, 3-(acetyloxy)-3-methyl-)	.. 587
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{C}(\text{O})\text{OCH}_3$	(Propanoic acid, 2-(acetyloxy)- 2-methyl-, methyl ester)	 587
$\text{cy-CH}_2\text{C}(\text{CH}_2\text{CH}_3)_2\text{CH}_2\text{O}$	(Oxetane, 3,3-diethyl-)	 587
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$	(1-Butanol, 3-methyl-, acetate)	 587
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2 + \text{O}_2(\text{a}^1\Delta_g)$		 587
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{CH}_2\text{CH}_3$	(2-Butanol, 2-methyl-, acetate)	 587
$\text{CH}_3\text{C}(\text{O})\text{OCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2$	(2-Butanol, 3-methyl-, acetate)	 588
$(\text{CH}_3)_2\text{CHC}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Propanoic acid, 2-methyl-, 1-methyl ethyl ester)	 588
$\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OC}(\text{CH}_3)_3$	(Propanoic acid 1,1-dimethylethyl ester)	.. 588
$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Butanoic acid 1-methylethyl ester)	.. 588
$\text{CH}_3\text{CH}_2\text{CH}_2\text{OC}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_3$	(Carbonic acid dipropyl ester)	 588
$(\text{CH}_3)_2\text{CHOC}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Carbonic acid bis(1-methylethyl) ester)	 588
$(\text{CD}_3)_2\text{CHOC}(\text{O})\text{OCH}(\text{CD}_3)_2$	(Carbonic acid bis(1-methyl-d ₃ - ethyl-2,2,2-d ₃) ester)	 589
$\text{CH}_3\text{OCH}_2\text{C}(\text{O})\text{OC}(\text{CH}_3)_3$	(Acetic acid, methoxy-, 1,1-dimethylethyl ester)	 589
$\text{CH}_3\text{OC}(\text{O})\text{OC}(\text{CH}_3)_2\text{CH}_2\text{CH}_3$	(Carbonic acid 1,1-dimethylpropyl methyl ester)	 589
$\text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{OOH}$	(Hydroperoxide, heptyl-)	 589
$\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{OOH})\text{CH}_3$	(Hydroperoxide, 1-methylhexyl-)	 590

$\text{C}_7\text{H}_x\text{S}_y$ -COMPOUND Reactions:

$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{SCH}_2\text{CH}=\text{CH}_2$	(Butane, 1-(2-propenylthio)-)	 590
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$\text{C}_7\text{H}_x\text{N}_y$ -COMPOUND Reactions:

$(\text{CH}_3)_3\text{CN}=\text{NCH}_2\text{CH}=\text{CH}_2$	(Diazene, (1,1-dimethylethyl)-2-propenyl)	590
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$\text{C}_7\text{H}_x\text{O}_y\text{N}_z$ -COMPOUND Reactions:

$(\text{CH}_3)_2\text{NC}(\text{O})\text{OC}(\text{CH}_3)_3$	(Carbamic acid, dimethyl-, 1,1-dimethylethyl ester)	 590
$(\text{CH}_3)_2\text{NC}(\text{O})\text{OC}(\text{CD}_3)_3$	(Carbamic acid, dimethyl-, (1,1-dimethyl-d ₉) ester)	 590

C_8H_x -COMPOUND Reactions:

$\text{cy-CH}=\text{CHCH}=\text{CHC}(\text{=CH}_2)\text{C}(\text{=CH}_2)$	(1,3-Cyclohexadiene, 5,6-bis(methylene)-)	 591
$\text{CH}_2=\text{C}=\text{CHCH}_2\text{CH}_2\text{CH}=\text{C}=\text{CH}_2$	(1,2,6,7-Octatetraene)	 591
$\text{CH}_2=\text{CHC}(\text{=CH}_2)\text{C}(\text{=CH}_2)\text{CH}=\text{CH}_2$	(1,5-Hexadiene, 3,4-bis(methylene)-)	 591
$\text{cy-C}(\text{CH}=\text{CH}_2)\text{C}(\text{CH}=\text{CH}_2)\text{CH}_2\text{CH}_2$	(Cyclobutene, 1,2-diethenyl-)	... 591
$\text{cy-CHC}(\text{=CH}_2)\text{C}(\text{=CH}_2)\text{CHCH}_2\text{CH}_2$	(1,4-Cyclohexanediyl, 2,3-bis(methylene)-)	 592

bicy-C ₈ H ₁₀ (Bicyclo[4.2.0]octa-1,5-diene)	592
bicy-C ₈ H ₁₀ (Bicyclo[2.2.0]hexane, 2,3-bis(methylene)-)	592
bicy-C ₈ H ₁₀ (Bicyclo[2.2.2]octa-2,5-diene)	593
trans,trans,trans-CH ₃ CH=CHCH=CHCH=CHCH ₃ (2,4,6-Octatriene, (E,E,E)-)	593
cis,cis-cy-CH=CHCH ₂ CH ₂ CH=CHCH ₂ CH ₂ (1,5-Cyclooctadiene, (Z,Z)-)	593
cy-CH=CHCH ₂ CH(CH=CH ₂)CH ₂ CH ₂ (Cyclohexene, 4-ethenyl-)	594
(+)-cy-CH=CHCH ₂ CH(CH=CD ₂)CH ₂ CH ₂ (Cyclohexene, 4-(ethenyl-2,2-d ₂)-, (R)-)	594
cy-C(CH ₂ CH ₃)=CHCH ₂ CH=CHCH ₂ (1,4-Cyclohexadiene, 1-ethyl-) ...	595
cy-C(CH ₃)=C(CH ₃)CH ₂ CH=CHCH ₂ (1,4-Cyclohexadiene, 1,2-dimethyl-)	595
trans-cy-CH(CH=CH ₂)CH(CH=CH ₂)CH ₂ CH ₂ (Cyclobutane, 1,2-diethenyl, trans-)	595
cis-cy-CH(CH ₃)CH(CH ₃)C(=CH ₂)C(=CH ₂) (Cyclobutane, 1,2-dimethyl-3,4-bis(methylene)-, cis-)	595
trans-cy-CH(CH ₃)CH(CH ₃)C(=CH ₂)C(=CH ₂) (Cyclobutane, 1,2-dimethyl-3,4-bis(methylene)-, trans-) ...	596
bicy-C ₈ H ₁₂ (Bicyclo[2.2.2]oct-2-ene)	596
CH ₃ C≡CCH ₂ CH ₂ CH(CH ₃) ₂ (2-Heptyne, 6-methyl-)	596
CH ₃ CH ₂ CH(CH ₃)CH ₂ C(CH ₃)=CH ₂ (1-Hexene, 2,4-dimethyl-)	597
(CH ₃) ₃ CC(CH ₃) ₂ CH ₂ (Butyl, 2,2,3,3-tetramethyl-)	597
n-C ₈ H ₁₈ (n-Octane)	597
(CH ₃) ₂ CH(CH ₂) ₄ CH ₃ (Heptane, 2-methyl-)	597
(CH ₃) ₃ CC(CH ₃) ₃ (Hexamethylethane)	598

C₈H_xO_y-COMPOUND Reactions:

bicy-C ₈ H ₁₀ O (Bicyclo[3.2.0]hept-3-en-6-one, 5-methyl-)	599
CH ₂ CH=CH ₂ OC(O)C(O)OCH ₂ CH=CH ₂ (Ethanedioic acid di-2-propenyl ester)	599
CH ₂ =CHCH=CHC(CH ₃) ₂ COOH (3,5-Hexanedioic acid, 2,2-dimethyl-)	599
CH ₂ =CHCH=CHC(CH ₃) ₂ COOD (3,5-Hexanedioic acid-d, 2,2-dimethyl-)	599
(cy-CH ₂ CH ₂ CH=CHCH ₂ CH)OC(O)CH ₃ (3-Cyclohexen-1-ol acetate) ...	599
CH ₃ C(O)OCH ₂ CH ₂ CH ₂ CH ₂ CH=CH ₂ (5-Hexen-1-ol acetate)	600
CH ₃ C(O)OCH ₂ CH ₂ CH=C(CH ₃) ₂ (3-Penten-1-ol, 4-methyl-, acetate)	600
CH ₃ C(O)OC(CH ₃) ₂ CH ₂ CH=CH ₂ (4-Penten-2-ol, 2-methyl-, acetate)	600
(cy-C ₆ H ₁₁)OC(O)CH ₃ (Acetic acid cyclohexyl ester)	600
bicy-C ₈ H ₁₄ O (Cyclobutanone, 3-ethoxy-2,2-dimethyl-)	600
[cy-CH ₂ CH ₂ C(CH ₃)]C(CH ₃) ₂ COOH (Cyclopropaneacetic acid, α,α,1-trimethyl)	601
cis-syn-[cy-CH(CH ₃)CH(CH ₃)CH]C(O)OCH ₃ (Cyclopropanecarboxylic acid, 2,3-dimethyl-, ethyl ester, (1α,2α,3α)-)	601
trans-[cy-CH(CH ₃)CH(CH ₃)CH]C(O)OCH ₃ (Cyclopropanecarboxylic acid, 2,3-dimethyl-, ethyl ester, (1α,2α,3β)-)	601
CH ₃ C(O)OC(CH ₃) ₂ CH ₂ COCH ₃ (2-Pentanone, 4-(acetyloxy)-4-methyl-)	601
CH ₃ CH ₂ CH ₂ CH ₂ C(O)OCH(CH ₃) ₂ (Pentanoic acid 1-methylethyl ester)	601
CH ₃ C(O)OCH ₂ CH ₂ C(CH ₃) ₃ (1-Butanol, 3,3-dimethyl-, acetate) ...	602
CH ₃ C(O)OCH(CH ₃)C(CH ₃) ₃ (2-Butanol, 3,3-dimethyl-, acetate) ..	602

$(\text{CH}_3)_2\text{CHCH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Butanoic acid, 3-methyl-, 1-methylethyl ester)	 602
$(\text{CH}_3)_3\text{CC}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Propanoic acid, 2,2-dimethyl-, 1-methylethyl ester)	 602
$\text{CH}_3\text{OC}(\text{O})\text{O}(\text{CH}_2)_5\text{CH}_3$	(Carbonic acid hexyl methyl ester)	 602
$\text{CH}_3\text{OC}(\text{O})\text{OCH}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	(Carbonic acid methyl 1-methylpentyl ester)	 602
$(\text{CH}_3)_3\text{COOC}(\text{CH}_3)_3$	(Peroxide, bis(1,1-dimethylethyl)-)	 603

$\text{C}_8\text{H}_x\text{S}_y$ -COMPOUND Reactions:

$(\text{CH}_3)_3\text{CSC}(\text{CH}_3)_3$	(Propane, 2,2'-thiobis[2-methyl-])	 603
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$\text{C}_8\text{H}_x\text{N}_y$ -COMPOUND Reactions:

$(\text{CH}_3)_2\text{CHCH}_2\text{N}=\text{NCH}_2\text{CH}(\text{CH}_3)_2$	(Diazene, bis(2-methylpropyl)-)	... 603
$(\text{CH}_3)_3\text{CN}=\text{NC}(\text{CH}_3)_3$	(Diazene, bis(1,1-dimethylethyl)-)	 603

C_9 -COMPOUND Reactions:

bicy- C_9H_{12}	(1H-Indene, 2,3,4,7-tetrahydro-)	 604
exo-bicy- C_9H_{14}	(Bicyclo[2.2.2]oct-2-ene, 5-methyl-, ($1\alpha, 4\alpha, 5\alpha$)-)	 604
endo-bicy- C_9H_{14}	(Bicyclo[2.2.2]oct-2-ene, 5-methyl-, ($1\alpha, 4\alpha, 5\beta$)-)	 604
bicy- $\text{C}_9\text{H}_8\text{O}$	(o-Quinodimethane)	 605
bicy- $\text{C}_9\text{H}_{12}\text{O}$	(Bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, ($1\alpha, 2\beta, 4\alpha$)-)	 605
bicy- $\text{C}_9\text{H}_{12}\text{O}$	(Bicyclo[3.2.0]hept-2-en-6-one, 7,7-dimethyl-)	 605
trans-[cy- $\text{CH}(\text{CH}_3)(\text{CH}_2)_4\text{CH}]\text{OC}(\text{O})\text{CH}_3$	(Cyclohexanol, 2-methyl-, acetate, (1R-trans)-)	 605
cis-[cy- $\text{CH}(\text{CH}_3)(\text{CH}_2)_4\text{CH}]\text{OC}(\text{O})\text{CH}_3$	(Cyclohexanol, 2-methyl-, acetate, (1S-cis)-)	 606
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{CH}_2\text{CH}(\text{CH}_3)_2$	(2-Pentanol, 2,4-dimethyl-, acetate)	 606
$\text{CH}_3\text{C}(\text{O})\text{OCH}(\text{CH}_3)\text{CH}_2\text{C}(\text{CH}_3)_3$	(2-Pentanol, 4,4-dimethyl-, acetate)	606
$\text{CH}_3\text{C}(\text{O})\text{OCH}(\text{CH}_2\text{CH}_3)\text{C}(\text{CH}_3)_3$	(3-Pentanol, 2,2-dimethyl-, acetate)	606
$\text{CH}_3\text{C}(\text{O})\text{OC}[\text{CH}(\text{CH}_3)_2](\text{CH}_3)\text{CH}_2\text{CH}_3$	(3-Pentanol, 2,3-dimethyl-, acetate)	 607
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{C}(\text{CH}_3)_3$	(2-Butanol, 2,3,3-trimethyl-, acetate)	607
$(\text{CH}_3)_3\text{CC}(\text{O})\text{OC}(\text{CH}_3)_3$	(Propanoic acid, 2,2-dimethyl-, 1,1-dimethylethyl ester)	 607
$(\text{CH}_3\text{CH}_2)_2\text{CHC}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Butanoic acid, 2-ethyl-, 1-methylethyl ester)	 607
$(\text{CH}_3)_3\text{CCH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Butanoic acid, 3,3-dimethyl-, 1-methylethyl ester)	 607
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Pentanoic acid, 2-methyl-, 1-methylethyl ester)	 607

$\text{CH}_3(\text{CH}_2)_4\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$ (Hexanoic acid 1-methylethyl ester)	.. 607
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OC}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (Carbonic acid dibutyl ester)	607
$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{OC}(\text{O})\text{OCH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ (Carbonic acid bis(1-methylpropyl) ester)	 608
$(\text{CH}_3)_2\text{CHCH}_2\text{OC}(\text{O})\text{OCH}_2\text{CH}(\text{CH}_3)_2$ (Carbonic acid bis(2-methylpropyl) ester)	 608
$(\text{CH}_3)_3\text{COC}(\text{O})\text{OC}(\text{CH}_3)_3$ (Carbonic acid bis(1,1-dimethylethyl) ester)	 608
$(\text{CH}_2=\text{CHCH}_2)_3\text{N}$ (Triallylamine)	 609
$[\text{cy}-(\text{CH}_2)_5\text{CH}]\text{NHCH}_2\text{CH}=\text{CH}_2$ (Cyclohexanimine, N-2-propenyl-)	... 609

C₁₀ to C₁₅-COMPOUND Reactions:

$(\text{cy}-\text{CH}=\text{CHCH}_2\text{CH}_2\text{C})=(\text{CCH}_2\text{CH}_2\text{CH}=\text{CH}-\text{cy})$ (Cyclopentene, 3-(4-Cyclopenten-1-ylidene)- (trans form))	 609
anti-cis-tricy-C ₁₀ H ₁₂ (Tricyclo[5.3.0.0 ^{2,6}]deca-3,9-diene; anti-cis-[2+2]-Dicyclopentadiene)	 609
endo-tricy-C ₁₀ H ₁₂ (Tricyclo[5.2.1.0 ^{2,6}]deca-3,8-diene, endo-)	610
exo-tricy-C ₁₀ H ₁₂ (-tricy-clo[5.2.1.0 ^{2,6}]deca-3,8-diene, exo-)	610
anti-tricy-C ₁₀ H ₁₂ (Tricyclo[4.2.1.1 ^{2,5}]deca-3,7-diene, (1 α ,2 β ,5 β ,6 α)-)	 610
$\text{CH}_2=\text{C}=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{C}=\text{CH}_2$ (1,2,8,9-Decatetraene)	 611
bicy-C ₁₀ H ₁₄ (Bicyclo[4.2.2]deca-3,7-diene)	 611
bicy-C ₁₀ H ₁₄ (Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-, (1 α ,4 α ,5 α)-)	 612
bicy-C ₁₀ H ₁₄ (Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-, (1 α ,4 α ,5 β)-)	 613
n-C ₁₀ H ₂₂ (n-Decane)	 613
(bicy-C ₆ H ₉)C(CH ₃) ₂ COOH (Bicyclo[3.1.0]hexane-1-acetic acid, α,α -dimethyl-)	 614
trans-cy-(CH ₂) ₄ CH[OC(O)CH ₃]CH[OC(O)CH ₃] (1,2-Cyclohexanediol diacetate, trans-)	 615
cis-cy-(CH ₂) ₄ CH[OC(O)CH ₃]CH[OC(O)CH ₃] (1,2-Cyclohexanediol diacetate, cis-)	 615
$\text{CH}_3\text{COOCH}[\text{C}(\text{CH}_3)_3]\text{CH}_2\text{CH}=\text{CH}_2$ (5-Hexen-3-ol, 2,2-dimethyl-, acetate)	 615
$[\text{cy}-\text{CH}_2\text{CH}(\text{CH}_3)\text{C}(\text{CH}_2\text{CH}_3)]\text{C}(\text{CH}_3)_2\text{COOH}$ (Cyclopropaneacetic acid, 1-ethyl- α,α ,2-trimethyl-)	 616
$\text{CH}_3\text{COOCH}[\text{CH}(\text{CH}_3)_2]\text{C}(\text{CH}_3)_3$ (3-Pentanol, 2,2,4-trimethyl-, acetate)	 616
$(\text{CH}_3)_3\text{CCH}_2\text{COOC}(\text{CH}_3)_3$ (Butanoic acid, 3,3-dimethyl-, 1,1-dimethylethyl ester)	 616
$\text{C}_6\text{H}_5\text{CH}_2\text{SCH}_2\text{CH}=\text{CH}_2$ (Benzene, [(2-propenylthio)methyl]-; Allyl benzyl sulfide)	 616
(bicy-C ₇ H ₁₁)C(CH ₃) ₂ COOH (Bicyclo[4.1.0]heptane-1-acetic acid, α,α -dimethyl-)	 617
endo-tricy-C ₁₂ H ₁₆ (endo-Tricyclo[6.2.2.0 ^{2,7}]dodeca-3,9-diene)	617
n-C ₁₂ H ₂₆ (n-Dodecane)	 617

[cy-(CH ₂) ₆ CH=C]C(CH ₃) ₂ COOH	(1-Cyclooctene-1-acetic acid, α,α-dimethyl-)	618
(CH ₃) ₂ CC(O)O[CH(CH ₂) ₅ -cy]	(Propanoic acid, 2,2-dimethyl-, cyclohexyl ester)	618
CH ₃ CH ₂ C(CH ₃) ₂ OOC(CH ₃) ₂ CH ₂ CH ₃	(Peroxide, bis(1,1-dimethylpropyl)-)	618
(CH ₃ CH ₂ CH ₂) ₂ CHCOOCH(CH ₃) ₂	(Pentanoic acid, 2-propyl-, 1-methylethyl ester)	618
CH ₃ CH ₂ C(CH ₃) ₂ OCOOC(CH ₃) ₂ CH ₂ CH ₃	(Carbonic acid bis(1,1-dimethylpropyl) ester)	618
trans-cy-(CH ₂) ₄ CH[OC(O)CH ₃]CH[C(CH ₃) ₃]	(Cyclohexanol, 2-(1,1-dimethylethyl)-acetate, trans-)	619
cis-cy-(CH ₂) ₄ CH[OC(O)CH ₃]CH[C(CH ₃) ₃]	(Cyclohexanol, 2-(1,1-dimethylethyl)-acetate, cis-)	619
trans-cy-(CH ₂) ₂ CH[OC(O)CH ₃](CH ₂) ₂ CH[C(CH ₃) ₃]	(Cyclohexanol, 4-(1,1-dimethylethyl)-acetate, trans-)	620
cis-cy-(CH ₂) ₂ CH[OC(O)CH ₃](CH ₂) ₂ CH[C(CH ₃) ₃]	(Cyclohexanol, 4-(1,1-dimethylethyl)-acetate, cis-)	620
CH ₃ C(O)O[CH(CH ₃) ₂ CH ₂ CH ₂ CH(CH ₃)CH ₂ -cy]	(Cyclohexanol, 5-methyl- 2-(1-methylethyl)-acetate, (1α,2β,5β)-)	621
(bicy-C ₈ H ₁₃)C(CH ₃) ₂ COOH	(Bicyclo[5.1.0]octane-1-acetic acid, α,α-dimethyl-)	621
(bicy-C ₉ H ₁₅)C(CH ₃) ₂ COOH	(Bicyclo[6.1.0]nonane-1-acetic acid, α,α-dimethyl-)	622
CH ₃ (CH ₂) ₅ OC(O)O(CH ₂) ₅ CH ₃	(Carbonic acid dihexyl ester)	623
CH ₃ (CH ₂) ₃ CH(CH ₃)OC(O)OCH(CH ₃)(CH ₂) ₃ CH ₃	(Carbonic acid bis(1-methylpentyl) ester)	623
CH ₃ (CH ₂) ₅ CH ₂ OOCH ₂ (CH ₂) ₅ CH ₃	(Peroxide, diheptyl-)	623
n-C ₁₅ H ₃₂	(n-Pentadecane)	623

4. Table of Chemical Kinetic Data for Combustion Chemistry

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + O + O → O₂ + O(¹S)						
Oxygen atom						
76 SLA/BLA1	EX	200-302	5.08(17)	0	654±302	3 3.07
O + O (+ M) → O₂ (+ M)						
Oxygen atom						
72 TCH	EX	298	3.63(15)			3
M = O ₂ .						
Room temperature, assumed to be 298 K.						
73 CAM/GRA ¹⁾	EX	196	(1.74±0.13)(15)			3
73 CAM/GRA ¹⁾	EX	298	(4.05±0.17)(15)			3
¹⁾ M = N ₂ .						
O + O₂ + O₂ → O₃ + O₂(¹A_g)						
Oxygen atom + Oxygen molecule						
71 FIN/SNE	DE	283-321	3.16(11)	0	1681	3
k ₁ = k ₋₁ K.						
O + O₂ (+ M) → O₃ (+ M)						
Oxygen atom + Oxygen molecule						
71 ELL/CAS	RL	298	5.5(-3)			2/2
M = He, Ar, Xe, N ₂ (at 253.7nm.)						
k _{ref} : O + O ₃ → O ₂ + O ₂ .						
71 HIP/TRO	EX	298	1.0(12)			2 1.2
Limiting high-pressure k.						
72 CAS/SCH ¹⁾	RL	261	2.67(-2)			2/2
72 CAS/SCH ¹⁾	RL	298	5.5(-3)			2/2
¹⁾ M = O ₂ , O ₃ , N ₂ (at 334 nm.)						
k _{ref} : O + O ₃ → O ₂ + O ₂ .						
73 STE/NIK1	RL	298	(1.08±0.12)(-3)			2/2
M = N ₂ + O ₂ . k _{ref} : O + NO ₂ → O ₂ + NO.						
The rate ratio is given by the expression						
k[M]/k _{ref} , therefore it is dimensionless.						
73 CAS/SCH ²⁾	RL	261	2.67(-2)			2/2
73 CAS/SCH ²⁾	RL	298	5.5(-3)			2/2
²⁾ M = O ₂ , N ₂ (at 334 nm.)						
k _{ref} : O + O ₃ → O ₂ + O ₂ .						
73 GAE/GLA	RN	300	6.0(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 GAE/TRO M = N ₂ . Limiting high-pressure k. Reevaluation.	EX	296	(1.7±0.7)(12)			2	
75 HIF/SCH Limiting high-pressure k.	RN	295	(1.7±0.7)(12)			2	
71 HIF/TRO M = N ₂ . Low-pressure k. Rate constant expressed as: k/[N ₂].	EX	298	2.9(14)			3	1.2
71 PRA/KAR O ₂ Photolysis. P(M) = (3-5) torr. k _{ref} : O + O ₂ + O ₂ → O ₃ + O ₂ . Efficiencies for the rate ratio are: 1.0(O ₂), (0.6±0.2)(Ar or He), (0.8±0.2)(Xe), (1.1±0.2)(N ₂), (3.2±0.5)(CO ₂).	RL	293	1.0			3/3	
71 PRA/MAK M = CO. Photolysis of O ₂ + CO mixture. P(O ₂) = 40 Tor. P(CO) = (1-60) torr. k _{ref} : O + CO → CO ₂ .	RL	293	(2.17±0.42)(7)			3/2	
71 STU/NIK1 M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 1.19(O ₂), 1.24(CO).	EX	300	2.00(14)			3	1.25
72 TCH M = O ₂ . Room temperature, assumed to be 298 K.	EX	298	4.35(14)			3	
72 HUI/HER1 M = Ar.	EX	200-346	(2.38±0.21)(13)	0	-510±23	3	
72 HUI/HER1 M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 1.7(N ₂).	EX	218	2.57(14)			3	
72 HUI/HER1 M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 0.92(He), 1.6(N ₂).	EX	298	1.32(14)			3	
73 BAL/LAR M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), Ar(0.78), 1.09(O ₂).	EX	295	(1.97±0.42)(14)			3	
73 BAL/LAR Average of present results and all the previous data. M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), Ar(0.68), 0.94(O ₂).	SE	295	(2.10±0.28)(14)			3	
73 BEV/JOH M = O ₂ . M-efficiencies relative to O ₂ are: 1.00(O ₂), 0.50(Ar), 2.41(N ₂), 2.46(CO ₂), 5.74(SF ₆).	EX	295	(1.96±0.11)(14)			3	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
73 ROS/TRA M = O ₂ , or N ₂ . k _{ref} : O ₃ [†] + M → O ₃ + M.	RL	300	9.03(3)			3/2	
74 ROS/TRA M = O ₂ , or N ₂ . Limiting high-pressure k.	EX	300	(1.14±0.20)(14)			3	
74 SNE M = O ₂ .	EX	295	(1.8±0.18)(14)			3	
75 HIP/SCH Limiting low-pressure k. Rate constant ex pressed as k/[N ₂]. M = N ₂ . Reevaluation.	RN	295	(2.3±1.0)(14)			3	
76 HOG/BUR M = O ₂ . Computer fit of data.	DE	300	(2.27±0.34)(14)			3	
77 ARE/SAM Discharge flow. M = O ₂ .	EX	298	1.20(14)			3	
79 ARN/COM ³⁾ M = Ar.	EX	263-298	(2.26±0.56)(13)	0	-525±70	3	
79 ARN/COM ³⁾ M = O ₂ .	EX	262-318	(2.45±0.16)(13)	0	-635±18	3	
79 ARN/COM ³⁾ M = N ₂ .	EX	263-309	(6.60±0.83)(12)	0	-995±37	3	
³⁾ O ₃ laser-pulse-photolysis. Resonance- absorption.							
80 KLA/AND ⁴⁾ M = O ₂ . n = 0 assumed.	EX	219-368	7.80(13)	0	-345±60	3	
80 KLA/AND ⁴⁾ M = O ₂ .	EX	219-368	(2.53±0.36)(14)	-1.25	0	3	
80 KLA/AND ⁴⁾ M = O ₂ .	EX	298	2.47(14)			3	1.15
80 KLA/AND ⁴⁾ M = N ₂ . n = 0 assumed.	EX	219-368	3.20(13)	0	-575±60	3	
80 KLA/AND ⁴⁾ M = N ₂ .	EX	219-368	(2.28±0.33)(14)	-2.0	0	3	
80 KLA/AND ⁴⁾ M = N ₂ .	EX	298	2.21(14)			3	1.15
80 KLA/AND ⁴⁾ M = Ar. n = 0 assumed.	EX	219-368	2.29(13)	0	-535±70	3	
80 KLA/AND ⁴⁾ M = Ar.	EX	219-368	(1.43±0.18)(14)	-1.9	0	3	
80 KLA/AND ⁴⁾ M = Ar.	EX	298	1.38(14)			3	1.15
80 KLA/AND ⁴⁾ M = Air. n = 0 assumed.	EX	219-368	3.38(13)	0	-525±60	3	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 KLA/AND ⁴) M = Air.	EX	219-368	(2.31±0.34)(14)	-1.9	0	3
80 KLA/AND ⁴) M = Air.	EX	298	2.25(14)			3 1.15
⁴) Flash-photolysis. Resonance-fluorescence. Arrhenius preexponential factor expressed as P(T/298) ⁿ in all the expressions with n ≠ 0.						
80 LAL/VER M = Ar. Pulsed photolysis of an O ₂ /Ar mixture. Resonance-fluorescence. P = 1 torr.	EX	298	(2.36±0.73)(14)			3
80 SUG/ISH1 M = He. Pulse-radiolysis. Resonance-absorption. P = (50-950) torr.	EX	296	(9.07±1.08)(13)			3
82 LIN/LEU ⁵) M = N ₂ . n = 0 assumed.	EX	218-366	(1.75±0.43)(13)	0	-731±67	3
82 LIN/LEU ⁵) M = N ₂ .	EX	218-366	(2.11±0.07)(14)	-2.62	0	3
82 LIN/LEU ⁵) M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.99(O ₂), 0.69(Ar), 0.60(He).	EX	298	(2.09±0.09)(14)			3
82 LIN/LEU ⁵) M = O ₂ . n = 0 assumed.	EX	227-353	(2.27±0.38)(13)	0	-668±46	3
82 LIN/LEU ⁵) M = O ₂ .	EX	227-353	(2.20±0.13)(14)	-2.37	0	3
82 LIN/LEU ⁵) M = Ar. n = 0 assumed.	EX	220-353	(1.29±0.50)(13)	0	-703±102	3
82 LIN/LEU ⁵) M = Ar.	EX	220-353	(1.41±0.10)(14)	-2.54	0	3
⁵) Flash-photolysis. Resonance-fluorescence. Arrhenius preexponential factor expressed as (T/298) ⁿ in all the expressions with n ≠ 0.						
O + O ₃ → O ₂ + O ₂ Oxygen atom + Ozone						
71 KRE/SIM k _{ref} : O + COS → SO + CO.	RL	197-299	6.4(-1)	0	-101	2/2
71 KRE/SIM	RN	197-299	7.23(12)	0	2164±101	2
72 BAL/EGO	EX	292-370	7.07(12)	0	1933±86	2 1.29
72 HUS/KIR1	RN	300	(7.83±3.01)(9)			2
72 MCC/KAU	EX	269-409	(6.32±1.08)(12)	0	2169±50	2
72 MCC/KAU	EX	298	(4.52±0.36)(9)			2
73 DAV/WON	EX	220-353	(1.22±0.11)(13)	0	2276±106	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 DAV	EX	293	(7.23±0.12)(9)			2
77 SHA The Arrhenius preexponential factor expressed as $A(T/298)^{0.75}$.	ES	250-2000	1.33(12)	0.75	1575	2
78 WES/WES Resonance fluorescence. Upper-limit k. O ₃ is in the vibrational symmetric and asymmetric stretching modes: O ₃ (100,001). P = (0-100) torr.	EX	298	≤9.03(12)			2
79 ARN/COM O ₃ laser-pulse-photolysis. Resonance-absorption.	EX	262-335	(1.28±0.11)(13)	0	2337±26	2
80 TOB/ULL M = CO ₂ . Conventional vacuum system. P < 1.0×10 ⁻⁵ torr.	RL	348-433	1.0(4)	0	1610±7055	2/2 39.8
$O(^1D) + O_3 \rightarrow O_2 + O_2$ (or $O + O + O_2$)						
Oxygen atom + Ozone						
71 GOL/GRE ¹⁾ At 228.8 nm.	RL	298	(4.1±0.9)			2/2
71 GOL/GRE ¹⁾ At 253.7 nm.	RL	298	(2.6±0.4)			2/2
¹⁾ k _{ref} : $O(^1D) + N_2O \rightarrow N_2 + O_2$ (a) → NO + NO (b)						
72 LIS/HEI ²⁾ k _{ref} : $O(^1D) + N_2 \rightarrow O(^3P) + N_2$. At 228.8, or 280.0 nm.	RL	298	(1.25±0.41)(1)			2/2
72 LIS/HEI ²⁾ k _{ref} : $O(^1D) + N_2 \rightarrow O(^3P) + N_2$. At 253.7 nm.	RL	298	(9.09±2.02)			2/2
72 LIS/HEI ²⁾ k _{ref} : $O(^1D) + CO_2 \rightarrow O(^3P) + CO_2$ At 228.8, or 253.7 nm.	RL	298	(2.50±0.83)			2/2
72 LIS/HEI ²⁾ k _{ref} : $O(^1D) + CO_2 \rightarrow O(^3P) + CO_2$. At 280 nm.	RL	298	(2.0±0.5)			2/2
²⁾ O ₃ Photolysis. From the reported reverse rate ratios.						
73 HEI/HUS1	EX	300	(1.62±0.12)(14)			2
73 HEI/HUS1 k _{ref} : $O(^1D) + O_2 \rightarrow$ products.	RL	300	3.9			2/2
73 HEI/HUS3 Time-resolved UV atomic Absorption-spectroscopy.	EX	300	(1.63±0.12)(14)			2
75 GAU/SNE k _{ref} : $O(^1D) + O_2 \rightarrow O + O_2(^1\Sigma_g^+)$.	RL	300	(8.0±2.0)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 GAU/SNE	RN	300	3.55(14)			2	
76 DAV/SAD	RL	298	2.0			2/2	
$k_{\text{ref}}: \text{O}(^1\text{D}) + \text{CO}_2 \rightarrow \text{O} + \text{CO}_2$.							
76 DAV/SAD	EX	298	(1.45±0.03)(13)			2	
76 STR/HOW	EX	103-393	1.45(14)	0	0	2	1.1
78 DAV/SCH ³⁾	EX	300	(1.45±0.22)(14)			2	
78 DAV/SCH ³⁾	EX	103-393	1.45(14)	0	0	2	
³⁾ Quadrupled-laser photolysis.							
$\text{O} + \text{H} (+ \text{M}) \rightarrow \text{OH}(\text{A}^2\Sigma^+, v=n) (+ \text{M})$							
Oxygen atom + Hydrogen atom							
76 KOI/MOR	ES	1250-2000	1.0(9)	0	5536	3	
M = Ar. n = 0.							
76 TIC	EX	298	2.71(1)			2	
n = 1.							
76 TIC	EX	298	5.80(11)			3	
M = H. n = 0.							
76 TIC	EX	298	6.17(9)			3	
M = H ₂ . n = 0.							
76 TIC	EX	298	1.45(10)			3	
M = H. v = 1.							
82 HID/TAK	EX	1200-3200	1.2(13)	0	3493	3	
H ₂ /O ₂ mixtures in Ar diluent, heated behind reflected shock-waves. n = 0. P _O = (50-100 torr).							
82 KOI/MOR1	EX	1250-3450	8.32(13)	0	4177±604	3	1.48
Reaction of O and H atoms in Argon diluent. O and H atoms generated by dissociation of O ₂ and H ₂ molecules in Ar, behind incident shock-waves. P _O = (6-30) torr. n = 0.							
$\text{O} + \text{H}_2 \rightarrow \text{OH} + \text{H}$							
Oxygen atom + Hydrogen molecule							
71 BRA/BEL1	EX	1200-1600	2.96(13)	0	4932±654	2	1.53
72 SCH/GET	RL	1700-2000	(4.0±1.0)			2/2	
$k_{\text{ref}}: \text{H} + \text{O}_2 \rightarrow \text{OH} + \text{O}$							
72 SCH/GET	RN	1700	4.5(12)			2	
73 GET	RN	1400-1900	3.2(14)	0	7549	2	1.25
74 NAM/TRO	EX	839-924	7.23(10)			2	
E _a not determined. Within the given T-range, k increases from 7.23×10 ¹⁰ to 1.33×10 ¹¹ cm ³ mol ⁻¹ s ⁻¹ .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
74 RAW/GAR2 k _{ref} : OH + OH → H ₂ O + O.	RL	1200-2000	2.9	0	3248	2/2	
74 RAW/GAR2	RN	1200-2000	1.6(14)	0	6808	2	
74 SCH/GET k _{ref} : O ₂ + H → O + OH	RL	1400-1900	(3.60±0.72)			2/2	
74 SCH/GET	RN	1400-1900	2.2(14)	0	6916±2406	2	1.25
75 BIR/KAS Upper-limit k. H ₂ is vibrationally excited with v' = 1.	EX	300	≤6.0(10)			2	
75 CAM/HAN2	EX	363-490	(3.1±0.5)(13)	0	4950±300	2	
75 DUB/MCK Air-afterglow.	EX	347-832	(5.30±3.01)(12)	0	4198±241	2	
75 DUB/MCK Resonance-fluorescence.	EX	347-832	(4.99±2.29)(12)	0	4330±241	2	
78 LIG ¹) OH is in ground state. Upper-limit k.	EX	302	≤2.83(9)	*		2	
78 LIG ¹) OH is either in ground state or vibrationally excited with v'' = 1.	EX	302	(6.02±5.42)(9)			2	
78 LIG ¹) OH is vibrationally excited with v'' = 1.	EX	302	(6.02±3.61)(9)			2	
¹) Flow-tube with tunable dye laser. H ₂ is vibrationally excited with v' = 1. P(Total) = 3 torr.							
80 BAS/KOG ²) n = 0 assumed.	EX	450-1160	1.51(13)	0	4479±201	2	1.26
80 BAS/KOG ²)	EX	450-1160	6.56(12)	0.5	4127±191	2	1.26
80 BAS/KOG ²) Extended T-range expression. Given with caution.	EX	293-1160	8.21(7)	6.4	302±332	2	100.
²) Combustion of H ₂ + O ₂ mixtures in a jet reactor. Gas-chromatography. Arrhenius preexponential factor expressed as: A(T/298) ⁿ in the expressions with n ≠ 0.							
80 LIG/MAT Flow-tube apparatus. Laser-induced Fluorescence. P = 3 torr.	EX	298	(5.5±3.0)(6)			2	
82 PAM/SKI1 Reaction of O with H ₂ behind reflected shock-waves, using H ₂ /N ₂ O/Ar mixtures. [O] _{max} = (1.7-6.6)×10 ¹³ molec.cm ⁻³ . P = (920-1224) torr.	EX	1919-2781	2.3(14)	0	6916	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 PAM/SKI2 Reaction of O with H ₂ behind reflected shock-waves, in H ₂ /O ₂ /Ar mixtures. Resonance-absorption spectroscopy. P = (1.16-2.67) atm. [O] = (5.42x10 ⁸ -3.49x10 ¹²) molec.cm ⁻³ .	EX	1000-2500	4.2(14)	0	6916	2
O + D₂ → OD + D						
Oxygen atom + Deuterium molecule						
75 APP/APP Arrhenius preexponential factor expressed as: A(T/298) ¹ .	ES	1700-3100	1.22(13)	1.0	8254	2 2.0
82 PAM/SKI1 Reaction of O with D ₂ behind reflected shock-waves, using H ₂ /N ₂ O/Ar mixtures. [O] _{max} = (1.9-7.2)x10 ¹³ molec.cm ⁻³ . P = (920-1224) torr.	EX	2097-2481	1.6(14)	0	7169	2
82 PAM/SKI2 Reaction of O with D ₂ behind reflected shock-waves, in D ₂ /O ₂ /Ar mixtures. Resonance-absorption spectroscopy. P = (1.16-2.67) atm. [O] = 5.42x10 ⁸ -3.49x10 ¹² molec.cm ⁻³ .	EX	1000-2500	1.9(14)	0	7169	2
O(¹D) + H₂ → OH + H						
Oxygen atom + Hydrogen molecule						
73 HEI/HUS2	EX	300	(1.63±0.18)(14)			2
73 HEI/HUS2 k _{ref} : O(¹ D) + N ₂ O → products.	RL	300	1.23			2/2
75 GAU/SNE k _{ref} : O(¹ D) + O ₂ → O + O ₂ (¹ Σ _g ⁺)	RL	300	(4.0±1.0)			2/2
75 GAU/SNE	RN	300	1.81(14)			2
75 STI/PAY k _{ref} : O(¹ D) + O ₂ → O(³ P) + O ₂	RL	300	(4.23±1.80)			2/2
75 STI/PAY	RN	300	(1.51±0.90)(14)			2
76 DAV/SAD k _{ref} : O(¹ D) + CO ₂ → O(³ P) + CO ₂ .	RL	298	1.08			2/2
76 DAV/SAD	RN	298	(7.83±0.30)(13)			2
77 DAV/SCH k _{ref} : O(¹ D) + CO ₂ → O(³ P) + CO ₂ .	RL	298	9.9(-1)			2/2
77 DAV/SCH	RN	298	(5.96±1.81)(13)			2
78 DAV/SCH ¹)	EX	300	(7.83±1.17)(13)			2
78 DAV/SCH ¹)	EX	204-35	5.96(13)	0	0	2

¹) Quadrupled-laser photolysis.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 PRA/PAU Photolysis of O ₂ /H ₂ mixtures diluted in He. P(O ₂) >15 torr. P(He) = 600 torr. k _{ref} = O(¹ D) + O ₂ → O(³ P) + O ₂	RL	298	(5.27±0.31)			2/2	
82 OGR/SWO Flash-photolysis of O ₂ /O ₃ /H ₂ mixtures in a vacuum system. P(Total) = 100 torr.	EX	298	(6.5±0.5)(13)			2	
O(¹ D) + D ₂ → OD + D							
Oxygen atom + Deuterium molecule							
73 HEI/HUS2	EX	300	(1.08±0.12)(14)			2	
76 DAV/SAD k _{ref} : O(¹ D) + CO ₂ → O(³ P) + CO ₂ .	RL	298	1.08			2/2	
76 DAV/SAD	RN	298	(7.83±0.30)(13)			2	
O + OH → O ₂ + H							
Oxygen atom + Hydroxyl							
76 KRI OH is in vibrational state v=9.	EX	298	1.81(13)			2	
77 CAM/HAN k _{ref} : CO + OH → CO ₂ + H	RL	425	(2.60±0.20)(2)			2/2	
77 CAM/HAN	RN	425	(2.65±0.52)(13)			2	
77 SPE/END ¹)	EX	295	(5.42±1.81)(13)			2	
77 SPE/GLA ¹)	EX	295	(6.32±3.19)(13)			2	
¹) OH is in vibrational state v=1.							
80 HOW/SMI Discharge-flow reactor. H ₂ O Flash-photolysis. Resonance-fluorescence. P(Total) = 3.75 torr.	EX	298	(2.29±0.54)(13)			2	
80 LEW/WAT ²) n = 0 assumed.	EX	221-499	(1.21±0.11)(1	0	-112±29	2	
80 LEW/WAT ²) The preexponential factor expressed as: A(T/298) ^{-0.362} .	EX	221-499	1.82(13)	-0.36	0	2	1.52
²) Discharge-flow-Resonance-fluorescence. [O] = (1-7)×10 ¹² molec.cm ⁻³ . [NO] ~ 1.5×10 ¹¹ molec.cm ⁻³ .							
81 HOW/SMI Discharge-flow system. OH formed by Flash-photo- lysis of H ₂ O. O atoms formed by reacting N with NO. Resonance-fluorescence. The preexponential factor expressed as: A(T/298) ^{-0.50} . [O] = (0.5-6.0)×10 ¹³ molec.cm ⁻³ .	EX	250-515	(2.32±0.08)(13)	-0.50	0	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O + HO₂ → OH + O₂							
Oxygen atom + Hydroperoxo							
73 PEE/MAH1	ES	1600	≈5.0(13)				2
77 BUR/HAR	EX	293	(2.13±0.60)(13)				2
77 SHA	ES	250-2000	8.25(12)	0.75	0		2
The preexponential factor expressed as: A(T/298) ^{0.75} .							
78 CAM/ROG	RL	425	(3.5±1.5)(1)				2/2
k _{ref} : H + HO ₂ → products. Discharge-flow reactor. P(Total) = (0.2-0.5) kPa.							
78 PRE	EX	293	(1.5±0.5)(13)				2
Laser Magnetic Resonance Spectrometry.							
79 BUR/CLI	EX	298	(1.87±0.60)(13)				2
Conventional discharge-flow system.							
79 HAC/PRE2	EX	298	(2.0±0.6)(13)				2
Isothermal discharge-flow reactor. ESR-LMR-spectrometry. P(He) < 10 mbar.							
80 LII/SAU	EX	298	(4.21±1.20)(13)				2
Electron pulse-radiolysis. Kinetic Spectrophotometry. P(Total) = 1200 torr.							
82 KEY2 ¹⁾	EX	229-372	(1.86±0.24)(13)	0	-200±28		2
82 KEY2 ¹⁾	EX	299	(3.67±0.24)(13)				2
¹⁾ Discharge-flow. Resonance-fluorescence. HO ₂ generated by reacting F with H ₂ O ₂ , or Cl with an excess of CH ₃ OH and O ₂ . O atoms produced by dissociating O ₂ in a microwave-discharge. P = 1 torr. [HO ₂] = (0.7-3.3)×10 ¹² molec.cm ⁻³ . [O] ₀ = (0.4-1.9)×10 ¹¹ molec.cm ⁻³ .							
82 SRI/QIU	EX	296	(3.25±0.54)(13)				2
Discharge-flow reactor. Laser-induced-fluorescence. UV-resonance-fluorescence. HO ₂ radicals generated by reacting F with H ₂ O ₂ . F atoms generated by dissociation of CF ₄ in a microwave-discharge. H and O atoms generated by dissociation of H ₂ and O ₂ in a microwave-discharge. [H] ₀ = [O] ₀ ~ (4-5)×10 ¹⁰ molec.cm ⁻³ . [CF ₄] = (1-10)×10 ¹³ molec.cm ⁻³ . [H ₂ O ₂] = 8×10 ¹² molec.cm ⁻³ . [NO] ~ 2×10 ¹⁴ molec.cm ⁻³ . P(He) ~ 2.5 torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O + H_2O \rightarrow H + HO_2$ (a) $\rightarrow OH + OH$ (b)						
Oxygen atom + Water						
79 HAC/PRE1 k_a . Isothermal flow. Laser Magnetic Resonance-Spectrometry. M = He. $k_1 = Kk_{-1}$. P(Total) = (130-800) Pa.	DE	298	7.4(-30)			2
71 ALB/HOY k_b .	EX	753-1045	4.0(13)	0	8707±252	2
$O(^1D) + H_2O \rightarrow O_2 + H_2$ (a) $\rightarrow OH + OH$ (b) $\rightarrow OH^* + OH$ (c)						
Oxygen atom + Water						
80 ZEL/WAG k_a/k_b . Reaction of Oxygen atoms with Water vapor. Flash-photolysis. $O(^1D)$ atoms generated by photolysis of Ozone. $P(O_3) = 0.6$ torr. $P(H_2O) = (2-4)$ torr. $P(He) = (8-11)$ torr.	RL	298	≤1.5(-2)			2/2
71 SCO/CVE k_b/k_{ref} . k_{ref} : $O(^1D) + N_2O \rightarrow N_2 + O_2$ (a) $\rightarrow NO + NO$ (b)	RL	296	(1.50±0.06)			2/2
72 FOR/SNE k_b/k_{ref} . k_{ref} : $O(^1D) + N_2 \rightarrow O + N_2$	RL	295	(3.5±1.5)			2/2
72 SIM/HEI2 k_b/k_{ref} . Estimated ratio. k_{ref} : $O(^1D) + CO \rightarrow O(^3P) + CO$	RL	300-423	3.79(-1)	0	-624	2/2
73 HEI/HUS1 k_b .	EX	300	(1.81±0.18)(14)			2
73 HEI/HUS1 k_b/k_{ref} . k_{ref} : $O(^1D) + O_2 \rightarrow$ products.	RL	300	4.4			2/2
73 HEI/HUS3 k_b . Time-resolved UV atomic Absorption-spectroscopy.	EX	300	(1.81±0.18)(14)			2
73 SIM/HEI2 k_b/k_{ref} . k_{ref} : $O(^1D) + N_2O \rightarrow N_2 + O_2$ (a) $\rightarrow NO + NO$ (b)	RL	373	(2.1±0.3)			2/2
75 GAU/SNE k_b/k_{ref} . k_{ref} : $O(^1D) + O_2 \rightarrow O + O_2(^1\Sigma_g^+)$	RL	300	(5.0±1.5)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 GAU/SNE k_b .	RN	300	2.23(14)			2	
76 DAV/SAD k_b/k_{ref} . $k_{ref}: O(^1D) + CO_2 \rightarrow O + CO_2$.	RL	298	1.75			2/2	
76 DAV/SAD k_b .	RN	298	(1.26±0.60)(13)			2	
76 STR/HOW k_b .	EX	253-353	1.39(14)	0	0	2	1.1
77 DAV/SCH k_b/k_{ref} . $k_{ref}: O(^1D) + CO_2 \rightarrow O(^3P) + CO_2$.	RL	298	2.3			2/2	
77 DAV/SCH k_b .	RN	298	(1.39±0.24)(14)			2	
72 LIS/HEI k_b/k_{ref} . Ozone Photolysis. $k_{ref}: O(^1D) + O_3 \rightarrow O_2 + O_2^*$	RL	298	1.5			2/2	
78 DAV/SCH ¹⁾	EX	300	(1.26±0.19)(14)			2	
78 DAV/SCH ¹⁾ ¹⁾ k_b . Quadrupled-laser photolysis.	EX	253-353	1.39(14)	0	0	2	
79 LEE/SLA k_b . O_2 -pulsed photolysis.	EX	300	(1.57±0.30)(14)			2	
81 GER/COM k_b . UV-Flash-photolysis Ozone in presence of H_2O vapor. $P(H_2O) = (2.5-19)$ torr. $P(O_3) = 1.5$ torr.	EX	298	(1.22±0.25)(14)			2	
81 PRA/PAU k_b/k_{ref} . Photolysis of O_2/H_2O mixtures diluted in He. $P(O_2) > 15$ torr. $P(He) = 600$ torr. $k_{ref} = O(^1D) + O_2 \rightarrow O(^3P) + O_2$.	RL	298	(6.7±0.4)			2/2	
71 PRA/VIL ²⁾ k_c/k_{ref} . $k_{ref}: O(^1D) + M \rightarrow O + M$.	RL	293	(2.0±0.5)(1)			2/2	
71 PRA/VIL ²⁾ k_c . Lower limit k .	RN	293	≥1.2(14)			2	
²⁾ Photolysis of an $O_2 + H_2O$ mixture. $P(O_2) = (30-100)$ Tor.							
71 PAR/CVE ³⁾ $k_{ref}: O(^1D_2) + O_2 \rightarrow$ products.	RL	298	1.07(1)			2/2	
71 PAR/CVE ³⁾ $k_{ref}: O(^1D_2) + N_2 \rightarrow$ products.	RL	298	9.64			2/2	
71 PAR/CVE ³⁾ $k_{ref}: O(^1D_2) + CO_2 \rightarrow$ products.	RL	298	2.98			2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
71 PAR/CVE ³⁾ k _{ref} : O(¹ D ₂) + (CH ₃) ₄ C → products. ³⁾ (k _a + k _b + k _c)/k _{ref} . Photolysis of N ₂ O/ Neopentane/SF ₆ mixtures. P(Total) ~ 320 torr.	RL	298	3.76(-1)			2/2
O + H ₂ O ₂ → OH + HO ₂ (a) (predominant path) → H ₂ O + O ₂ (b)						
Oxygen atom + Hydrogen peroxide						
71 ALB/HOY k _a + k _b .	EX	370-800	2.8(13)	0	3221±302	2
74 DAV/WON k _a + k _b .	EX	283-368	(1.66±0.25)(12)	0	2125±261	2
82 ROS k _a + k _b . (Recommended expression). Conventional fast-flow system. O atoms generated by reacting N with NO in a microwave discharge. Mass-spectrometry. P[H ₂ O ₂] ₀ = (0.3-1.5)×10 ¹⁸ molec.cm ⁻³ . P = (0.9-1.7) torr.	SE	302-349	(1.66±0.25)(12)	0	2125±261	2
O(¹ D) + H ₂ O ₂ → OH + HO ₂						
Oxygen atom + Hydrogen peroxide						
76 FLE/HUS	EX	300	(3.13±0.36)(14)			2
O + SO (+ M) → SO ₂ (+ M)						
Oxygen atom + Sulfur monoxide						
71 MIY/TAK1 M = Ar.	EX	298	(7.40±0.73)(16)			3
79 GRI/REE M = Ar. Reflected shock-waves. k ₁ = k ₋₁ K. The preexponential factor expressed as: A(T/298) ^{-1.84} .	DE	300-3880	3.36(17)	-1.84	0	3
O + SO ₂ (+ M) → O ₂ + SO (+ M) (a) → SO ₃ (+ M) (b)						
Oxygen atom + Sulfur dioxide						
80 GRI/REE k _a . Thermolysis of SO ₂ diluted in N ₂ O/Ar mixtures behind reflected shock-waves.	EX	2630-3570	(4.0±0.4)(12)	0	9210	2
80 SLA/GRI k _a . Shock-heated mixtures of SO ₂ /N ₂ O mixtures behind reflected shock-waves, in presence of Ar.	EX	3320-3760	(3.8±0.5)(11)	0	0	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 WES/DEH2 k _b . M = He. M-efficiencies relative to He are: 1.0(He), 2.4(N ₂), 9.5(SO ₂).	EX	297	(3.0±0.2)(14)			2	
75 WES/DEH2 k _b . M = He.	EX	248-415	(3.9±0.9)(16)	0	1400±50	2	
74 ATK/PIT3 k _b . M = N ₂ .	EX	299-392	3.32(16)	0	1007±201	3	
78 ATK/PIT4 ¹⁾ k _b . M = Ar.	EX	299-440	1.12(16)	0	1009±151	3	
78 ATK/PIT4 ¹⁾ k _b . M = Ar.	EX	299	(3.81±0.76)(14)			3	
78 ATK/PIT4 ¹⁾ k _b . M = SO ₂ .	EX	299	(3.45±1.09)(15)			3	
78 ATK/PIT4 ¹⁾ k _b . M = N ₂ .	EX	300	(4.97±0.98)(14)			3	
¹⁾ Flash-photolysis. NO ₂ chemiluminescence.							
79 AST/GLA k _b . M = Ar. Incident pr reflected shock-waves. [Ar] = (0.5-4.2)×10 ¹⁹ molec.cm ⁻³ . Rate constant expressed as k[Ar]. Based on: k ₁ = Kk ₋₁ .	DE	1700-2500	1.06(13)	0	-7870	3	
79 MER/LEV ²⁾ k _b /k _{ref} . k _{ref} : O + SO ₂ → O ₂ + SO ₂	RL	1685	6.6(3)			3/2	
79 MER/LEV ²⁾ k _b .	ES	2250	7.4(14)			3	
²⁾ Combustion in a quartz-tube burner. M = CH ₄ , N ₂ , O ₂ , H ₂ S.							
82 SMI/TSE k _b . Reaction of SO ₂ with O in a CO/O ₂ /Ar flame. Mass-spectrometry. P = 200 torr.	EX	1435-1850	4.4(14)	0	-3163	3	
O + SO ₃ (+ M) → O ₂ + SO ₂ (+ M)							
Oxygen atom + Sulfur trioxide							
71 MER/LEV k determined in H ₂ S flame.	EX	1100-1400	6.5(14)	0	5435	2	
71 MER/LEV k determined in COS flame.	EX	900-1600	2.8(14)	0	6039	2	
72 JAC/WIN Average of 8 experimental points.	EX	300	2.79(7)			2	
72 JAC/WIN Average of 7 experimental points.	EX	413	4.22(7)			2	
72 JAC/WIN Average of 6 experimental points.	EX	500	5.31(7)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
72 JAC/WIN A and B recalculated from the above three k's. The A-factor given in the initial abstract ($3.0 \times 10^{15} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$) should be 3.0×10^{16} .	ES	300-487	(1.40 ± 0.27)(8)	0	487 $\pm$ 79	2
79 MER/LEV Combustion in a quartz-tube burner.	RN	1685	1.5(11)			2
82 SMI/TSE Reaction of SO ₂ with O in a CO/O ₂ /Ar flame. Mass-spectrometry. P = 200 torr.	EX	1435-1850	1.32(12)	0	3070	2
75 WES/DEH1 M = He. M-efficiencies relative to He are: 1.0(He), 1.4(N ₂), <10.0(SO ₃).	EX	298	(7.3 ± 0.2)(17)			3
75 WES/DEH1 M = He.	EX	298-507	5.0(16)	0	-785	3
O + S ₂ O → SO + SO						
Oxygen atom + Sulfur oxide (S ₂ O)						
74 STE/ALV	ES	298	(9.03 ± 1.20)(11)			2
O + SH → H + SO						
Oxygen atom + Mercapto						
75 CUP/GLA	EX	295	(9.64 ± 3.01)(13)			2
O + H ₂ S → OH + SH (a)						
→ [H ₂ SO] [‡] → HSO + H (b)						
→ [H ₂ SO] [‡] → products (c)						
Oxygen atom + Hydrogen sulfide						
76 WHY/TIM k _a . Flash-photolysis. Resonance-fluorescence. Same data given in 78 WHY/TIM.	EX	263-495	(4.36 ± 0.64)(12)	0	1661 $\pm$ 50	2
78 SLA/BAI k _b . Fast flow-reactor. Photoionization Mass-spectrometer. A and B (not explicitly given) recalculated from the reported experimental data.	EX	281-497	(1.30 ± 0.36)(13)	0	1815 $\pm$ 139	2
79 SIN/IRW k _a + k _b + k _c . Phase-shift. Gas-chromatography.	EX	297-502	(1.56 ± 0.83)(13)	0	2171 $\pm$ 202	2
82 SIN/PAR ¹⁾ k _a /(k _a + k _b + k _c). Based on the reported lower-limit (0.52) and upper-limit (1.0) ratios.	RL	298	(7.6 ± 2.4)(-1)			2/2
82 SIN/PAR ¹⁾ k _b /(k _a + k _b + k _c). Upper-limit ratio.	RL	298	<2.0(-1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 SIN/PAR ¹⁾ k _c /(k _a + k _b + k _c). Upper-limit ratio. Product of path (c) cannot be HSOH. ¹⁾ Reaction of O with H ₂ S in a quartz cell, in N ₂ O/H ₂ /CO mixtures. O atom generated by Hg-sensi- tized decomposition of N ₂ O. Gas-chromatography. P(Total) = (368-743) torr. P(H ₂ S) = (5.5-21) torr. P(CO) = (50-200) torr.	RL	298	<4.8(-1)			2/2
O + D ₂ S → OD + SD Oxygen atom + Hydrogen sulfide (D ₂ S)						
76 WHY/TIM	EX	298-450	(6.32±3.43)(12)	0	2144±156	2
O + N (+ M) → NO (+ M) Oxygen atom + Nitrogen atom						
73 CAM/GRA ¹⁾	EX	196	(4.38±0.38)(15)			3
73 CAM/GRA ¹⁾	EX	298	(3.34±0.36)(15)			3
¹⁾ M = N ₂ .						
O + N ₂ (+ M) → NO + N (+ M) (a) → N ₂ O (+ M) (b) Oxygen atom + Nitrogen molecule						
73 BAC/EBE k _a .	EX	1900-2500	5.0(13)	0	37947	2 2.0
73 IVE/BAS k _a .	ES	1900-2400	1.3(14)	0	37947	2
76 HAR/NAS k _a . Best fit to the experimental data.	EX	2270-2620	(9.1±0.4)(13)	0	38000	2
77 BLA/SME k _a .	EX	1880-2350	7.5(13)	0	38249	2 1.2
77 MON/HAN2 k _a .	EX	2384-3850	1.84(14)	0	38374	2 1.35
79 MON/HAN k _a . Shock tube. IR-emission. CO-laser absorption.	EX	2384-3850	(1.84±0.64)(14)	0	38374	2
71 STU/NIK1 k _b . M = N ₂ . Upper-limit k.	EX	300	<1.81(10)			3
O(¹ D) + N ₂ (+ M) → N ₂ O (+ M) (a) → other products (b) Oxygen atom + Nitrogen molecule						
73 GAE/GLA k _a . Expressed as: k = [N ₂]1.0x10 ¹² cm ⁶ mol ⁻² s ⁻¹ .	ES	300	≈1.0(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 PRA/PAU k _b . Photolysis of O ₂ /N ₂ mixtures diluted in He. k _{ref} = O(¹ D) + O ₂ → O(³ P) + O ₂ . P(He) = 600 torr. P(O ₂) > 15 torr.	RL	298	(7.21±0.79)(-1)			2/2
72 SIM/LIS k _a . M = N ₂ . Upper-limit ratio. k _{ref} : O(¹ D) + M → O + M.	RL	298	<4.82(-2)			3/2
O + N ₃ → NO(A ² Σ ⁺) + N ₂ Oxygen atom + Azide						
79 PIP/KRE NaN ₃ thermolysis. Conventional flow-system.	EX	461	(6.02±2.41)(12)			2
O + NO (+ M) → O ₂ + N (+ M) (a) → NO ₂ (+ M) (b) Oxygen atom + Nitrogen oxide (NO)						
74 HAN/FLO k _a . The preexponential factor expressed as: A(T/298) ¹ .	EX	2500-4100	7.03(11)	1.0	19446	2
77 MCC/KRU ¹⁾	EX	1750-2100	5.13(11)	1.0	19446	2 1.26
77 MCC/KRU ¹⁾ Based on a curve-fit of all previous k's. Recommended k. Same data given in 76 MCC/KRU.	RE	1750-2100	1.11(12)	1.0	20851	2
¹⁾ k _a . Flow reactor. The preexponential factor expressed as: A(T/298) ¹ .						
73 GAE/GLA k _b . M = N ₂ . Limiting high-pressure k.	RN	300	8.0(12)			2
73 HAR/JOH k _b [M]/k _{ref} . M = N ₂ . k _{ref} : O + NO ₂ → O ₂ + NO.	RL	296	(1.8±0.1)(-1)			2/2
75 GAE/TRO k _b . M = N ₂ . Limiting high-pressure k.	EX	296	(1.8±0.3)(13)			2
75 HIP/SCH k _b . M = N ₂ . Limiting high-pressure k.	RN	295	(1.8±0.3)(13)			2
75 SIN/FUR k _b . M = N ₂ O.	EX	298-473	(6.12±0.45)(15)	0	-619±28	2
76 MIC/PAY k _b . M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 0.87(He), 0.73(Ne), 0.96(Kr), 1.64(N ₂) at 217 K. 1.0(Ar), 0.95(He), 0.80(Ne), 0.99(Kr), 1.66(N ₂) at 298 K. 1.0(Ar), 1.04(He), 0.89(Ne), 1.01(Kr), 1.68(N ₂) at 500 K.	EX	217-500	(3.27±0.42)(15)	0	-594±35	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
76 MIC/PAY k _b . M = He.	EX	217-500	(3.91±0.44)(15)	0	-523±30	2	
76 MIC/PAY k _b . M = Ne.	EX	217-500	(3.38±0.40)(15)	0	-518±30	2	
76 MIC/PAY k _b . M = Kr. n = 0 assumed.	EX	217-500	(3.45±0.40)(15)	0	-574±35	2	
76 WHY/MIC1 k _b . M = N ₂ .	EX	217-500	(5.62±0.73)(15)	0	-584±35	2	
76 WHY/MIC1 k _b . M = N ₂ . The preexponential factor expressed as: A(T/298) ^{-1.82}	EX	217-500	4.33(16)	-1.82	0	2	
77 ATK/PER1 k _b . M = Ar.	EX	298-439	5.30(15)	0	-473±101	2	
77 ATK/PER1 k _b . M = Ar.	EX	298	(2.55±0.25)(16)			2	
71 ATK/CVE k _b . M = N ₂ O.	EX	298	(3.7±0.8)(16)			3	
71 STU/NIK1 k _b . M = He. M-efficiencies relative to He are: 1.0(He), 2.26(NO).	EX	300	2.41(16)			3	1.1
71 STU/NIK2 k _b .	EX	300	2.47(16)			3	
72 ATK/CVE k _b . M = N ₂ O.	EX	298-473	(2.6±0.21)(15)	0	-805±151	3	
74 ATK/PIT1 k _b . M = N ₂ O.	EX	300-392	9.6(15)	0	-453±101	3	
74 ATK/PIT2 k _b . M = N ₂ O.	EX	300	(4.30±0.43)(16)			3	
74 FUR/ATK k _b . M = N ₂ O.	EX	298	(5.78±0.08)(16)			3	
75 CAM/HAN2 k _b . M = N ₂ . M-efficiencies relative to N ₂ are: 1.0(N ₂), 0.62(Ar).	EX	285-432	(1.8±0.5)(15)	0	-900±85	3	
75 HIP/SCH k _b . M = N ₂ . Limiting low-pressure k. Reevaluation. Rate constant expressed as k/[M]. M-effi- ciencies relative to N ₂ are: 1.00(N ₂), 0.65(He), 0.86(Ne), 1.28(Ar), 1.21(CO), 1.65(CO ₂), 1.66(SF ₆), 1.43(CH ₄), 1.15(C ₂ H ₆), 1.33(cy-C ₃ H ₈), 2.13(C ₃ F ₈), 1.36(2,2-Dimethylpropane), 1.36(2,2-Dimethylbutane), 1.68(Isopropylbromide).	RN	295	(2.7±0.5)(16)			3	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 AND k _b . M = Ar. NO Flash-photolysis. Time-resolved detection of NO ₂ chemiluminescence.	EX	298	(2.80±0.18)(16)			3	
78 ATK/PIT4 ²) M = SO ₂ .	EX	299	(9.43±3.27)(16)			3	
78 ATK/PIT4 ²) ²) k _b . Flash-photolysis. NO ₂ chemiluminescence.	EX	300	(3.99±0.73)(16)			3	
78 MIC/PAY1 k _b . M = N ₂ . Flash-photolysis.	EX	217-500	(5.62±0.73)(15)	0	-582±37	3	
79 AND/STE k _b . M = Ar. NO vacuum-UV Flash-photolysis. Time-resolved detection of NO ₂ chemiluminescence.	EX	237-397	(4.61±0.73)(15)	0	-508±50	3	
79 MIC/LEE ³) k _b . M = He. n = 0 assumed.	EX	217-500	(3.92±0.44)(15)	0	-523±30	3	
79 MIC/LEE ³) k _b . M = He.	EX	217-500	2.60(16)	-1.63	0	3	
79 MIC/LEE ³) k _b . M = Ar. n = 0 assumed.	EX	217-500	(3.27±0.42)(15)	0	-594±35	3	
79 MIC/LEE ³) k _b . M = Ar.	EX	217-500	2.50(16)	-1.86	0	3	
79 MIC/LEE ³) k _b . M = N ₂ . n = 0 assumed.	EX	217-500	(5.62±0.73)(15)	0	-584±35	3	
79 MIC/LEE ³) k _b . M = N ₂ .	EX	217-500	4.33(16)	-1.82	0	3	
³) Flash-photolysis. Resonance-fluorescence. The preexponential factor expressed as: A(T/298) ⁿ in all the expressions with n ≠ 0.							
80 SUG/ISH2 ⁴) k _b . M = N ₂ .	EX	298	(2.79±0.18)(16)			3	
80 SUG/ISH2 ⁴) k _b . M = He.	EX	298	(1.52±0.18)(16)			3	
⁴) Pulse-radiolysis technique. Resonance-absorption. P(Total) = (200-100) torr.							
82 FAI/SIN k _b . M _{eff} = 1.0(N ₂ O) and 31(CH ₃ OH). Modulated Phase-shift. O atoms generated by Hg-photosensitized decomposition of N ₂ O. Gas-chromatography.	EX	298	(9.79±2.71)(12)			3	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$O(^1D) + NO \rightarrow O_2 + N$							
Oxygen atom + Nitrogen oxide (NO)							
73 HEI/HUS2	EX	300	(5.12±0.60)(13)			2	
73 HEI/HUS2	RL	300	4.3(-1)			2/2	
$k_{ref}: O(^1D) + N_2O \rightarrow \text{products.}$							
$O + NO_2 (+M) \rightarrow O_2 + NO (+M) (a)$ $\rightarrow NO_3 (+M) (b)$							
Oxygen atom + Nitrogen oxide (NO ₂)							
72 CLY/CRU	EX	298	(3.67±0.36)(12)			2	
$k_a.$							
72 GER/DEM	EX	298	(4.0±1.0)(12)			2	
$k_a.$							
73 DAV/HER	EX	230-339	(5.49±0.27)(12)	0	0	2	
$k_a.$							
73 HAR/JOH	RN	296	5.54(12)			2	
$k_a.$							
73 SLA/WOO ¹⁾	EX	240	6.32(12)			2	1.15
73 SLA/WOO ¹⁾	EX	296	5.60(12)			2	1.15
¹⁾ $k_a.$							
74 BEM/CLY ²⁾	EX	298	(5.72±0.66)(12)			2	
74 BEM/CLY ²⁾	EX	298-1055	5.43(12)	-0.52	0	2	1.37
The preexponential factor expressed as: $A(T/298)^{-0.52}.$							
²⁾ $k_a.$							
74 STE/ALV	RL	298	(6.0±0.5)			2	
$k_a.$ $k_{ref}: O + S_2O \rightarrow SO + SO.$							
75 WU/NIK	EX	298	5.72(12)			2	
$k_a.$ NO ₂ Photolysis.							
73 GAE/GLA ³⁾	RN	300	6.0(12)			2	
75 GAE/TRO ³⁾	EX	296	(1.3±0.2)(13)			2	
³⁾ $k_b.$ M = N ₂ . Limiting high-pressure k.							
73 HAR/JOH	RL	296	(2.2±0.1)(-1)			2/2	
$k_b[M]/k_{ref}.$ M = N ₂ . $k_{ref}: O + NO_2 \rightarrow O_2 + NO.$							
75 HIP/SCH	RN	295	(1.3±0.2)(13)			2	
$k_b.$ M = N ₂ . Limiting high-pressure k. Reevaluation.							
73 HAR/JOH	RN	296	2.97(16)			3	
$k_b.$							
73 HUI ⁴⁾	EX	263	(1.45±0.44)(17)			3	
73 HUI ⁴⁾	EX	298	(7.62±2.18)(16)			3	
⁴⁾ $k_b.$ M = Ar.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 HIP/SCH M = N ₂ . Limiting low-pressure k. Reevaluation. k expressed as k/[M]. M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.94(He), 1.30(Ne), 1.38(Ar), 1.97(CO), 2.63(CO ₂), 3.60(SF ₆), 2.59(CH ₄), 2.67(C ₂ H ₆), 2.26(C ₃ H ₈), 3.15(cy-C ₃ H ₆), 4.36(CF ₄), 4.27(C ₂ F ₆), 7.11(C ₃ F ₈), 3.72(2,2-Dimethylpropane), 3.89(2,2-Dimethylbutane), 2.83(Isopropylbromide), 5.95(2,2,3-Trimethylbutane).	RN	295	(2.9±0.4)(16)			3
75 WU/NIK k _b . M = Ar. NO ₂ Photolysis.	EX	298	4.50(16)			3
O(¹ D) + NO ₂ → O ₂ + NO Oxygen atom + Nitrogen oxide (NO ₂)						
73 HEI/HUS2	EX	300	(1.39±0.12)(14)			2
73 HEI/HUS2 k _{ref} : O(¹ D) + N ₂ O → N ₂ + O ₂ (a) → NO + NO (b)	RL	300	1.05			2
75 GAU/SNE k _{ref} : O(¹ D) + O ₂ → O + O ₂ (¹ Σ _g ⁺) Estimated ratio.	RL	300	~4.0			2/2
75 GAU/SNE	RN	300	1.81(14)			2
O + NO ₃ → O ₂ + NO ₂ Oxygen atom + Nitrogen oxide (NO ₃)						
75 GRA	RN	298-329	(6.02±1.2)(12)	0	0	2
78 GRA/JOH Modulated photolysis technique.	EX	298	(6.02±0.24)(12)			2
O + N ₂ O → O ₂ + N ₂ (a) → NO + NO (b) Oxygen atom + Nitrogen oxide (N ₂ O)						
72 BOR/SKA k _a /k _b . Reflected shock waves. 20% N ₂ O + 80% Ar.	RL	1000-2000	(8.0±3.0)(-1)	0	0	2/2
72 SOL k _a .	SE	1000-3000	4.5(13)	0	12128	2
75 DOV/NIP k _a + k _b .	EX	2160-3400	5.25(13)	0	12557±1122	2 1.58
76 DEA k _a . Data-fit to a proposed mechanism. Same data given in 75 BAB/DEA.	ES	1950-3075	1.15(13)	0	12630	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
77 MON/HAN1 $k_a = k_b$. Best data-fit.	ES	1815-3365	6.23(13)	0	12350	2 1.65
77 BAL/VAN k_a . Supersonic molecular beam. Mass-spectrometer. P = 40 torr. Based on the k for the reaction: $O + N_2O \rightarrow NO + NO$.	EX	1900	(5.9±1.8)(11)			2
77 DEA/STE1 k_a . M = Ar. Shock-waves. $N_2O/CO/Ar$ mixtures at a Total concentration of $(2.5-7.7) \times 10^{18}$ molec.cm ⁻³ .	EX	2100-3200	4.64(13)	0	14073	2
80 SUL/KLI k_a . Thermolysis of N_2O behind shock-waves, diluted in Ar. P = (1300-3500) torr.	EX	1685-2000	(4.43±3.97)(13)	0	6215±1198	2
80 ZAS/LOS k_a . Thermolysis of (0.5-2.5)% N_2O in Ar, He, N_2 , or CO, behind shwaves. [M] = $(0.6-6.0) \times 10^{19}$ molec.cm ⁻³ .	EX	1700-2500	2.6(13)	0	11072	2
71 LIP ¹⁾	RL	1400-2000	(5.1±1.6)(-1)			2/2
73 LIP/MIL ¹⁾	RL	1300-1950	5.0(-1)			2/2
73 MIL/MAT ¹⁾ Average rate-ratio.	RL	1169-1650	(3.17±2.70)(-1)			2/2
76 MIL ¹⁾	RL	1216-1655	(2.52±1.35)(-1)			2/2
76 MIL ¹⁾ Average rate-ratio.	RL	1370-1655	2.75(-5)			2/2 2.45
¹⁾ k_b/k_a .						
72 SOL k_b .	SE	1000-3000	4.5(13)	0	12128	2
76 DEA k_b . fit to a proposed mechanism. Same data given in 75 BAB/DEA.	ES	1950-3075	1.15(13)	0	12630	2
77 BAL/VAN k_b . Supersonic molecular beam. Mass-spectrometer. P = 40 torr.	EX	1800-2000	(5.4±1.6)(14)	0	16105	2
77 DEA/STE1 k_b . M = Ar. Shoch waves.. $N_2O/CO/Ar$ mixtures. Conc.(Total) = $(2.5-7.7) \times 10^{18}$ molec.cm ⁻³ .	EX	2100-3200	4.64(13)	0	14073	2
80 SUL/KLI k_b . M = Ar. Thermolysis of N_2O behind reflected shock-waves. P = (1300-3500) torr.	EX	1685-2000	(4.07±3.26)(13)	0	6215±1198	2
80 ZAS/LOS k_b . Thermolysis of (0.5-2.5)% N_2O in Ar, He, N_2 , or CO behind shock-waves. [M] = $(0.6-6.0) \times 10^{19}$ molec.cm ⁻³ .	EX	1700-2500	1.4(14)	0	15098	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O(^1D) + N_2O \rightarrow O_2 + N_2$ (a) $\rightarrow NO + NO$ (b) $\rightarrow N + NO_2$ (c)						
Oxygen atom + Nitrogen oxide (N_2O)						
71 GOL/GRE ¹⁾ At 228.8 nm.	RL	298	(3.3±0.3)(-1)			2/2
71 GOL/GRE ¹⁾ At 253.7 nm.	RL	298	(3.7±0.3)(-1)			2/2
¹⁾ $k_a/(k_a + k_b)$.						
71 SCO/PRE k_a/k_b . Photolysis of NO_2 and N_2O mixtures.	RL	298	(1.01±0.06)			2/2
72 GRE k_a/k_b . For completely thermalized $O(^1D)$, $k_a/k_b = 0.85 \pm 0.05$.	RL	298	(5.9±0.1)(-1)			2/2
72 SIM/GRE k_a/k_b . Rate ratio valid for $O(^1D)$ atoms with translational energy in excess of 10 kcal/mole.	RL	298	(6.5±0.7)(-1)			2/2
72 SIM/GRE k_a/k_b . Rate ratio valid for $O(^1D)$ atoms with no excess thermal energy.	RL	300	(9.0±1.0)(-1)			2/2
73 GH/ELL k_a/k_b .	RL	298	(7.0±0.2)(-1)			2/2
74 WIE/PAR k_a/k_b .	RL	298	(1.0±0.17)			2/2
79 DAV/HOW ²⁾ k_a/k_b . UV-photolysis of pure N_2O .	RL	300	(6.80±0.18)(-1)			2/2
79 DAV/HOW ²⁾ k_a/k_b . UV-photolysis of N_2O + He mixtures.	RL	300	8.0(-1)			2/2
79 DAV/HOW ²⁾ ²⁾ Chemical-ionization mass spectrometry. ³⁾ $k_a/k_b = (0.72 \pm 0.11) + (21.6 \pm 7.0/T)$. Best data-fit.	RL	170-434	³⁾	³⁾	³⁾	2/2
79 MAR/BAH $k_a/(k_a + k_b + k_c)$. N_2O photolysis in excess He. Gas-chromatography.	RL	298	(6.17±0.15)(-1)			2/2
79 VOL/FEL ⁴⁾ k_a/k_b . Photolysis of pure N_2O . $P(N_2O) = (39-120)$ torr.	RL	290	(7.34±1.13)(-1)			2/2
79 VOL/FEL ⁴⁾ k_a/k_b . Photolysis of N_2O in He. $P(He) = (622-730)$ torr. $P(N_2O) = (29-97)$ torr.	RL	290	(9.19±1.00)(-1)			2/2
⁴⁾ Gas chromatography.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 PRA/FAU k_a/k_{ref} . Photolysis of O_2/N_2O mixtures diluted in He. $k_{ref} = O(^1D) + O_2 \rightarrow O(^3P) + O_2$. $P(He) = 600$ torr. $P(O_2) > 15$ torr.	RL	298	(4.6±0.3)			2/2
72 LIS/HEI ⁵⁾ At 228.8 nm.	RL	298	2.5(-1)			2/2
72 LIS/HEI ⁵⁾ At 253.7 nm. Approximate ratio.	RL	298	~4.0(-1)			2/2
72 LIS/HEI ⁵⁾ At 280 nm.	RL	298	6.7(-1)			2/2
⁵⁾ $(k_a + k_b)/k_{ref}$. O_3 photolysis. $k_{ref}: O(^1D) + O_3 \rightarrow O_2 + O_2$						
72 LOU/CVE ⁶⁾ $k_{ref}: O(^1D) + CO_2 \rightarrow O + CO_2$	RL	298	(1.25±0.14)			2/2
72 FAR/SYM ⁶⁾ $k_{ref}: O(^1D) + (CH_3)_4C \rightarrow$ products.	RL	298	(1.45±0.10)(-1)			2/2
73 GHO/ELL ⁶⁾ $k_{ref}: O(^1D) + O_2 \rightarrow O + O_2$.	RL	298	(3.23±0.10)			2/2
⁶⁾ $(k_a + k_b)/k_{ref}$.						
73 GHO/ELL $k_a + k_b$.	RN	298	1.2(14)			2
73 HEI/HUS2 $k_a + k_b$.	EX	300	(1.32±0.12)(14)			2
75 GAU/SNE $(k_a + k_b)/k_{ref}$. $k_{ref}: O(^1D) + O_2 \rightarrow O + O_2(^1\Sigma_g^+)$	RL	300	(3.3±0.5)			2/2
75 GAU/SNE $k_a + k_b$.	RN	300	1.45(14)			2
76 DAV/SAD ⁷⁾ $(k_a + k_b)/k_{ref}$.	RL	298	1.25			2/2
76 DAV/SAD ⁷⁾ $k_a + k_b$.	RN	298	(8.43±0.60)(13)			2
77 DAV/SCH ⁷⁾ $(k_a + k_b)/k_{ref}$.	RL	298	1.1			2/2
77 DAV/SCH ⁷⁾ $k_a + k_b$.	RN	298	(6.63±1.20)(13)			2
⁷⁾ $k_{ref}: O(^1D) + CO_2 \rightarrow O(^3P) + CO_2$.						
78 DAV/SCH ⁸⁾ $k_a + k_b$.	EX	300	(8.43±1.26)(13)			2
78 DAV/SCH ⁸⁾ $k_a + k_b$.	EX	204-359	6.63(13)	0	0	2
⁸⁾ Quadrupled-laser photolysis.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 LAM/HAS ⁷) (k _a + k _b)/k _{ref} .	RL	177	(2.9±0.4)			2/2
81 LAM/HAS ⁷) (k _a + k _b)/k _{ref} .	RL	296	(4.0±0.4)			2/2
81 LAM/HAS ⁷) k _b /k _{ref} .	RL	177-296	(6.2±0.9)(-1)			2/2
⁷) N ₂ O/N ₂ /He photolysis. P(Total) = (100-600) torr. k _{ref} : O(¹ D) + N ₂ → O(³ P) + N ₂ .						
71 SCO/PRE k _c /k _a . NO ₂ /N ₂ O photolysis. Upper-limit ratio.	RL	298	<5.0(-3)			2/2
O(¹ S) + N ₂ O → products						
Oxygen atom + Nitrogen oxide (N ₂ O)						
76 SLA/BLA2	EX	200-368	(2.29±0.60)(13)	0	423±75	2
O + N ₂ O ₅ → products						
Oxygen atom + Nitrogen oxide (N ₂ O ₅)						
75 GRA Upper-limit k.	RN	298	≤1.2(10)			2
78 GRA/JOH Modulated photolysis. Upper limit k.	EX	298	≤1.20(10)			2
78 KAI/JAP1 Discharge-flow. Upper-limit k. P(N ₂) = 4.5 torr.	EX	223-300	≤1.81(8)			2
O + NS → SO + N						
Oxygen atom + Nitrogen sulfide (NS)						
72 LIT/DAL	ES	300	~1.2(13)			2 2.0
O + NH ₂ → OH + NH (a) → H + HNO (b)						
Oxygen atom + Amidogen						
73 GEH/HOY k _a + k _b .	EX	298	2.1(12)			2
O + NH ₃ → OH + NH ₂						
Oxygen atom + Ammonia						
74 DOV/NIP Upper-limit k.	EX	1620-1920	≤1.0(13)	0	3322	2
74 KIR/MER Flow reactor. Ultrasonic molecular beam.	EX	300-450	(4.9±1.5)(12)	0	3091±108	2
80 LAL/VER O ₂ photolysis in Ar. Resonance-fluorescence.	EX	298	(3.01±0.90)(9)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O(¹D) + NH₃ → OH + NH₂							
Oxygen atom + Ammonia							
76 DAV/SAD	EX	298	(2.04±0.18)(14)				2
76 FLE/HUS	EX	300	(3.79±0.42)(14)				2
77 DAV/SCH	RL	298	2.5				2/2
k _{ref} : CO ₂ + O(¹ D) → CO ₂ + O(³ P).							
77 DAV/SCH	RN	298	(1.51±0.30)(14)				2
78 DAV/SCH ¹⁾	EX	300	(2.05±0.31)(14)				2
78 DAV/SCH ¹⁾	EX	204-354	1.51(14)	0	0		2
T-independent k.							
¹⁾ Quadrupled-laser photolysis.							
O + HNO → OH + NO							
Oxygen atom + Nitrosyl hydride							
75 CAM/HAN2	RN	425	≥1.13(2)				2/2
k _{ref} : H + HNO → H ₂ + NO. Lower-limit ratio.							
O + HONO → products							
Oxygen atom + Nitrous acid							
78 KAI/JAP2	EX	300-355	≤6.02(8)	0	0		2
Discharge-flow reactor. Upper-limit k.							
O + HONO₂ → OH + NO₃							
Oxygen atom + Nitric acid							
72 MOR/SMI	EX	300	<7.82(9)				2
Upper-limit k.							
74 CHA/WAY	EX	300	≤1.81(7)				2
Upper-limit k.							
O + HO₂NO₂ → products							
Oxygen atom + Peroxynitric acid							
81 CHA/TRE	EX	228-297	(4.22±7.36)(13)	0	3369±489		2
Low-pressure stirred-flow. Discharge-flow.							
Modulated molecular-beam Mass-spectrometer.							
P ~2 torr.							
O(¹D) + CO → CO₂							
Oxygen atom + Carbon monoxide							
73 HEI/HUS1 ¹⁾	EX	300	(4.40±0.42)(13)				2
73 HEI/HUS1 ¹⁾	RL	300	1.05				2/2
k _{ref} : O(¹ D) + O ₂ → products.							
¹⁾ Time-resolved UV atomic Absorption-spectroscopy.							
Same data given in 73 HEI/HUS3.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 PRA/PAU Photolysis of O ₂ /CO mixtures diluted in He. P(He) = 600 torr. $k_{\text{ref}} = \text{O}(^1\text{D}) + \text{O}_2 \rightarrow \text{O}(^3\text{P}) + \text{O}_2$	RL	298	(9.0±1.3)(-1)			2/2
O + CO (+ M) → CO₂ (+ M) (a)						
→ CO₂(³B₂) (+ M) (b)						
Oxygen atom + Carbon monoxide						
72 DEM k_a . M = CO ₂ . k increasing from 9.77x10 ⁷ to 3.5x10 cm ³ mol ⁻¹ s ⁻¹ between 0.74 and 42 atm. Hippler and Troe's expression used.	EX	298	9.77(7)			2
72 DEM k_a . M = CO ₂ . k increasing from 5.24x10 ⁷ to 2.75x10 ⁸ cm ³ mol ⁻¹ s ⁻¹ between 0.74 and 42 atm. Sauer's expression used.	EX	298	5.24(7)			2
72 SIM/HEI1 k_a . M = N ₂ O. Limiting high-pressure k.	EX	298-472	1.6(10)	0	1459	2
73 GAE/GLA k_a . M = CO. Limiting high-pressure k.	RN	300	≤3.0(8)			2
77 DEA/STE1 k_a . M = Ar. Shock/waves. N ₂ O/CO/Ar mixtures.	EX	2100-3200	(5.80±1.09)(13)	0	0	2
71 DON/HUS ¹⁾ k_a . M = Ar.	EX	300	(5.08±2.54)(12)			3
71 DON/HUS ¹⁾ k_a . M = He.	EX	300	(5.08±2.54)(12)			3
¹⁾ Kinetic Absorption-spectroscopy.						
71 MIY/TAK1 k_a . M = Ar.	EX	298	(2.11±0.61)(16)			3
71 STU/NIK1 k_a . M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.77(He), 1.45(CO).	EX	300	7.98(11)			3 1.25
72 BAL/JAC k_a . M = Ar.	ES	300-3500	3.0(14)	0	1510	3
72 SIM/HEI1 k_a . M = N ₂ O. Limiting low-pressure k.	EX	298-472	5.9(15)	0	2063	3
72 SLA/WOO k_a . M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 1.70(CO), 2.70(CO ₂).	EX	296	(8.34±1.45)(11)			3
72 SLA/WOO k_a . M = CO.	EX	250-370	2.36(15)	0	2184±277	3
72 ZAB/HAR k_a . Upper-limit k.	EX	1400-1500	≤2.0(14)			3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
73 INN k _a . M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 0.46(CO), 0.55(CO ₂).	EX	296	(3.56±0.73)(12)			3	
74 HAR/VAS k _a . M = Ar. Upper-limit k.	EX	1500	<2.0(14)			3	
74 INN k _a . M = CO ₂ .	EX	257-277	8.02(14)	0	1782±408	3	
74 KON k _a . M = O ₂ . Reevaluation.	SE	400-500	2.35(12)	0	-1862	3	
74 WAG/ZAB k _a . M = Ar. Limiting low-pressure k. The preexponential factor expressed as: A(T/298) ⁻¹⁵ .	RN	298-4000	1.96(15)	-1.5	2516	3	
76 WEI k _a . M = Ar(89%) + CO(4%) + O ₂ (3%) + NO ₂ (3%). The preexponential factor expressed as: A(T/298) ⁻¹ .	EX	2500-2900	1.01(16)	-1.0	2013	3	
78 HAR/GAR k _a . M = Ar. Reflected shock-waves. Best fit of experimental data. P(Total) = (2-4) atm.	EX	1300-2200	2.79(13)	0	-2285	3	
80 SUG/ISH1 ²) k _a . M = He.	EX	296	(3.63±0.73)(12)			3	
80 SUG/ISH1 ²) k _a . M = CO. ²) Pulse-radiolysis. Resonance-absorption. P = (50-950) torr.	EX	296	(1.09±0.73)(13)			3	
80 TOB/ULL k _b . M = CO ₂ . Vacuum system. P < 1.0x10 ⁻⁵ torr.	EX	348-433	1.26(9)	0	805±755	2	40.0
O + CO₂ (+ M) → O₂ + CO (+ M) (a)							
→ CO₃ (+ M) (b)							
Oxygen atom + Carbon dioxide							
74 BAB/DEA k _a .	EX	3015-4675	4.78(12)	0	18168±1459	2	1.58
71 STU/NIK1 k _b . M = CO. Upper-limit k.	EX	300	≤3.27(12)			3	
80 SUG/ISH1 k _b . M = He. Pulse-radiolysis. Resonance- absorption. P = (50-950) torr. Upper-limit k.	EX	296	<1.45(12)			3	
O(¹D) + CO₂ → O₂ + CO							
Oxygen atom + Carbon dioxide							
73 HEI/HUS1	EX	300	(1.26±0.12)(14)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
73 HEI/HUS1 k _{ref} : O ₂ + O(¹ D) → products.	RL	300	3.1			2/2
75 GAU/SNE k _{ref} : O(¹ D) + O ₂ → O + O ₂ (¹ Σ _g ⁺).	RL	300	(2.7±0.5)			2/2
75 GAU/SNE	RN	300	1.20(14)			2
81 PRA/PAU Photolysis of O ₂ /CO ₂ mixtures diluted in He. P(He) = 600 torr. k _{ref} = O(¹ D) + O ₂ → O(³ P) + O ₂ .	RL	298	(2.82±0.20)			2/2
O + CH → products						
Oxygen atom + Methylidyne						
81 MES/FIL CH produced by IR multiple photon dissociation of CH ₃ OH in Ar. Same data given in 80 MES/CAR. P(CH ₃ OH) = 1.3 mtorr. P(Ar) = (5-15) torr.	EX	298	(5.72±0.84)(13)			2
O + CH₂ → CO + H + H (a) → CHO + H (b)						
Oxygen atom + Methylene						
73 JON/BAY1 k _a /k _{ref} . k _{ref} : CH≡CH + CH ₂ → products.	RL	298	(3.1±0.2)			2/2
79 VIN/DEB2 k _a . Oxidation of Acetylene in a fast-flow reactor. P(Total) = 2.2 torr.	EX	295	(7.83±1.81)(13)			2
82 GRE/HOM1 k _a . Reaction of the CH≡CH/O/H system diluted with He/N ₂ in a discharge-reactor. Resonance-fluores- cence. O atoms generated by reacting N with O. H atoms produced by a discharge of the mixture H ₂ /He. Best fit to experimental data. P = 2 torr.	EX	298	(5.0±1.0)(13)			2
81 TSU/HAS k _b . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ mixtures in Ar behind reflected shock-waves.	ES	1200-1800	3.02(13)	0	0	2
O + CH₃ → H + HCHO						
Oxygen atom + Methyl						
72 NIK/MOR2	EX	300	5.42(13)			2
73 MOR/NIK1 Unreported T assumed to be 298K. Lower-limit k.	EX	298	>1.81(13)			2
73 PEE/MAH1 k _{ref} : OH + CH ₄ → H ₂ O + CH ₃	RL	1100-1900	4.4	0	-2013	2/2
73 PEE/MAH1	RN	1100-1900	1.3(14)	0	1007	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
73 WAS/BAY	EX	297	(7.4±0.15)(13)			2
74 SLA/FRU	EX	300	(1.11±0.17)(14)			2
75 BIO/LAZ	EX	1550-1725	1.05(14)	0	0	2
75 BOW1	ES	1900-2400	1.0(14)	0	0	2
Best data-fit.						
76 WAS/BAY	EX	259-341	(6.02±1.20)(13)	0	0	2
76 TSU	DE	1500-2000	6.03(13)	0	0	2
Computer calculation.						
71 CLA/IZO2	ES	1350	2.53(13)			2
Shock-waves. Time-of-flight Mass-spectrometry.						
Total conc. = 9×10^{13} molec.cm ⁻³ .						
71 DEA/KIS	DE	1750-2575	6.02(13)	0	0	2
Shock-waves. Best-fit to experimental data.						
Total conc. = 5×10^{17} molec.cm ⁻³ .						
72 MOR/NIK	EX	298	>1.81(13)			2
Discharge-flow. Ti-of-flight Mass-spectrometry. Lower-limit k.						
80 BHA/FRA	EX	1700-2300	(8.5±1.0)(13)	0	0	2
Shock-tube. Atomic Resonance-Absorption.						
80 WAS	EX	298	(8.31±2.77)(13)			2
Generation of CH ₃ by reaction of O with Ethene in a fast-flow reactor. Photoionization Mass-spectrometer. P(Total) = (1.9-3.7) torr. Comparable data in 79 WAS1, 79 WAS2 and 79 WAS3.						
82 PLU/RVA2	EX	295	(6.87±1.75)(13)			2
Reaction of CH ₃ with O in a flow-reactor, in He. CH ₃ generated by reacting F with CH ₄ . O and F atoms generated by dissociation of O ₂ and CF ₄ in a microwave discharge. Mass-spectrometry. [He] = (6.3-13.1) × 10 ¹⁶ molec.cm ⁻³ . [O] = (0.6-5.1) × 10 ¹² molec.cm ⁻³ . [CH ₄] = (5-10) × 10 ¹² molec.cm ⁻³ . [CF ₄] = (3-8) × 10 ¹¹ molec.cm ⁻³ .						
O + CH ₄ → OH + CH ₃ (a) → H ₂ O + CH ₂ (b)						
Oxygen atom + Methane						
71 AVR/KOL1	EX	373-583	(4.22±2.11)(13)	0	4630±352	2
k _a .						
71 DEA/KIS	DE	1750-2575	1.57(14)	0	4001	2
k _a . Shock-waves. Best-fit to experimental data. Total conc. = 5×10^{17} molec.cm ⁻³ .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 BRA/BRO k_a .	EX	1300-2000	1.9(14)	0	5900	2
77 ROT/JUS k_a .	EX	1500-2250	4.09(14)	0	7030	2
78 SHA k_a . The preexponential factor expressed as: $A(T/298)^2$.	DE	300-2500	4.55(11)	2.0	3240	2
79 FEL/FON k_a . Flash-photolysis. Resonance-fluorescence. High-temperature photolysis. The preexponential factor expressed as: $A(T/298)^{2.075}$. The reported k's are represented reasonably well by the above rate expression of Roth and Just, but are somewhat larger at higher T's.	EX	525-1250	1.59(12)	2.075	3840	2
80 FEL/FON k_a . High-T photochemistry reactor. Resonance-fluorescence. $P(N_2) = 25$ torr.	EX	1140	(5.60±0.48)(11)			2
80 KLE/TAN k_a . Flash-photolysis. Discharge-flow. Resonance-fluorescence. $P(Ar) = (100-200)$ torr.	EX	474-1156	(1.29±0.18)(14)	0	5472±97	2
80 ROT ¹⁾	EX	1500-2200	4.10(14)	0	7030	2
80 ROT ¹⁾ Modified Arrhenius expression over extended T-range by combining the k's of several authors. The preexponential factor expressed as: $A(T/298)^{2.075}$.	EX	300-2200	1.59(12)	2.075	3840	2
¹⁾ k_a . Thermolysis of N_2O behind shock-waves. Atomic Resonance-Absorption Spectrophotometry. Same data published in 79 ROT/JUS1.						
81 KLE/TAN ²⁾	EX	474-1156	(1.20±0.20)(14)	0	5435±112	2
81 KLE/TAN ²⁾ Arrhenius expression extended over the upper T-range, obtained by combining the present data with the results of two previous shock tube studies. The preexponential factor expressed as: $A(T/298)^{0.5}$.	EX	475-2250	(5.45±0.34)(13)	0.5	5179±54	2
²⁾ k_a . M = Ar. Resonance-fluorescence combined with either Flash-photolysis at a total P of (100-200) torr., or Discharge-flow at a total P of (1.1-2.9) torr.						
71 AVR/KOL1 k_b .	EX	373-583	(3.31±1.63)(12)	0	3372±352	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O(^1D) + CH_4 \rightarrow OH + CH_3$ (a) (Main channel)						
$\rightarrow H_2 + HCHO$ (b)						
Oxygen atom + Methane						
72 GRE	RL	298	(2.28±0.20)			2/2
k_a/k_{ref} . $k_{ref}: O(^1D) + N_2O \rightarrow O_2 + N_2$ (m)						
$\rightarrow NO + NO$ (n)						
For completely thermalized $O(^1D)$,						
$k_a/k_{ref} = 1.35 \pm 0.3$						
72 GRE/HEI	RL	298	(2.28±0.20)			2/2
k_a/k_{ref} . $k_{ref}: O(^1D) + N_2O \rightarrow O_2 + N_2$ (m)						
$\rightarrow NO + NO$ (n)						
With added He, $k_a/k_{ref} = (1.35 \pm 0.3)$						
73 HEI/HUS2	EX	300	(1.87±0.24)(14)			2
$k_a + k_b$.						
73 HEI/HUS2	RL	300	1.41			2/2
$(k_a + k_b)/k_{ref}$. $k_{ref}: O(^1D) + N_2O \rightarrow O_2 + N_2$ (m)						
$\rightarrow NO + NO$ (n)						
75 GAU/SNE	RL	300	(5.1±1.0)			2/2
$(k_a + k_b)/k_{ref}$. $k_{ref}: O(^1D) + O_2 \rightarrow O + O_2(^1\Sigma_g^+)$						
75 GAU/SNE	RN	300	2.29(14)			2
$k_a + k_b$.						
76 DAV/SAD	RL	298	1.08			2/2
$(k_a + k_b)/k_{ref}$.						
$k_{ref}: O(^1D) + CO_2 \rightarrow O(^3P) + CO_2$.						
76 DAV/SAD	RN	298	(7.83±1.81)(13)			2
$k_a + k_b$.						
76 JAY/SIM	RL	298	(1.1±0.2)(-1)			2/2
$k_b/(k_a + k_b)$.						
77 DAV/SCH	RL	298	1.4			2/2
$(k_a + k_b)/k_{ref}$.						
$k_{ref}: O(^1D) + CO_2 \rightarrow O(^3P) + CO_2$.						
77 DAV/SCH	RN	298	(8.43±2.41)(13)			2
$k_a + k_b$.						
78 DAV/SCH ¹⁾	EX	300	(7.83±1.17)(13)			2
78 DAV/SCH ¹⁾	EX	198-357	8.43(13)	0	0	2
T-independent k.						
¹⁾ k_a . Quadrupled-laser photolysis.						
81 PRA/PAU	RL	298	(6.85±0.13)			2/2
k_a/k_{ref} .						
Photolysis of O_2/CH_4 mixtures diluted in He.						
$k_{ref} = O(^1D) + O_2 \rightarrow O(^3P) + O_2$						
$P(O_2) > 15$ torr. $P(He) = 600$ torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + CHO → OH + CO (a)						
→ H + CO₂ (b)						
Oxygen atom + Methyl, oxo-						
73 MAC/THR $k_a/(k_a + k_b)$.	RL	300	5.4(-1)			2/2
76 KRI k_a . OH is in vibrational state $v = 9$.	EX	298	3.61(12)			2
72 WES/DEH3 k_b/k_a .	RL	298	(7.3±1.5)(-1)			2/2
73 MAC/THR $k_b/(k_a + k_b)$.	RL	300	4.6(-1)			2/2
74 WAS/MAR $k_a + k_b$. Ethylene used as source of CHO.	EX	297	(1.26±0.24)(14)			2
76 MAR $k_a + k_b$. Formaldehyde used as source of CHO.	EX	297	(1.33±0.24)(14)			2
O + ECHO → OH + CHO (a)						
→ OH + CO + H (b)						
→ H + H + CO₂ (c)						
→ products (d)						
Oxygen atom + Formaldehyde						
73 MAC/THR k_a .	EX	300	(9.0±1.0)(10)			2
79 KLE k_a . Flash-photolysis. Resonance-fluorescence. Mass-spectrometry.	EX	250-500	(1.67±0.19)(13)	0	1525±40	2
80 KLE/SKO k_a . Discharge-flow. Resonance-Fluorescence. k obtained by combining the present data with the data from reference 79 KLE (see above.)	EX	250-750	(1.77±0.16)(16)	0	1543±34	2
71 DEA/KIS k_b . Shock-waves. Best-fit to experimental data. Total conc. = 5×10^{17} molec.cm ⁻³ .	DE	1750-2575	6.02(13)	0	0	2
71 IZO/KIS k_b . Shock waves. Best-fit to experimental data. Total conc.: 5×10^{17} molec.cm ⁻³ .	DE	1400-2200	6.02(13)	0	0	2
81 MOR/HEI $k_c/(k_a + k_c)$. Photolysis NO ₂ in presence of CHO and O ₂ , at 360 nm. Upper-limit ratio. P(Total) = 52 torr.	RL	296	≤(1.6±0.2)(-1)			2/2
74 CAD/WIC k_d . Unspecified T-range near 300K.	EX	~300	3.7(12)	0	1208	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
74 CAD/WIC k_d .	EX	300	6.6(10)			2	
79 CHA/BAR k_d . Discharge-flow system. Mas-spectrometry.	EX	296-437	(2.29±0.48)(13)	0	1583±73	2	
O + CH₃OH → OH + CH₂OH (a)							
→ OH + CH₃O (b)							
Oxygen atom + Methanol							
71 AVR/KOL2 k_a .	EX	343-413	3.01(11)	0	1409±352	2	
75 BAS/KOG k_a . Reaction of O with CH ₃ OH vapor in a cylindrical reactor. O generated by decomposition of an O ₂ /He mixture in a high-frequency discharge. ESR-spectroscopy. Gas-chromatography.	EX	300-830	(4.28±0.07)(12)	0	1022±67	2	
76 OWE/ROS k_a . Initial step of a proposed mechanism. Flow-reactor.	EX	301-451	1.45(9)	0	1540±144	2	1.07
81 GRO/JUS k_a . Conventional fast-flow reactor. Time-of-flight Mass-spectrometry.	EX	300-1006	(3.43±1.14)(14)	0	2750±150	2	
81 KEI/TAN k_a . Discharge-flow. Flash-photolysis, or Resonance-fluorescence. P(Total) = (2.7-4.4) torr.	EX	298-998	(1.63±0.30)(13)	0	2531±81	2	
82 FAI/SIN k_a . Major path. Modulated Phase-shift. O atoms generated by Hg-photosensitized decomposition of N ₂ O. Gas-chromatography.	EX	297-544	(9.79±2.71)(12)	0	2267±111	2	
80 LAL/VER $k_a + k_b$. Pulsed photolysis of an O ₂ /Ar mixture. Resonance-fluorescence. P = 1 torr.	EX	298	(3.61±0.60)(7)			2	
71 AVR/KOL2 k_b .	EX	343-413	6.02(12)	0	3322±352	2	
72 LEF/MEA k_b .	EX	273-438	(1.70±0.66)(12)	0	1147±101	2	
O(¹D) + CH₃OH → products							
Oxygen atom + Methanol							
75 OSI/SIM k_{ref} : O(¹ D) + N ₂ O → NO + NO (a) → O ₂ + N ₂ (b) ($k_{ref} = k_a + k_b$)	RL	298-345	(5.5±2.0)	0	0	2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + CS → CO(v=n) + S						
Oxygen atom + Carbon monosulfide						
71 HAN/SMI v≤13.	ES	298	8.43(12)			2
72 HAN/RID k _{ref} : O + CS → CO(v=13) + S. Ratio increasing from 0.1 to 0.9 between between v=7 and v=12, then decreasing to 0.3 from v = 14 to v = 15. Unreported T assumed to be 298 K.	RL	298	~1.0(-1)			2/2
75 SLA/GRA1 Vibrational levels not indicated.	EX	305	(1.24±0.08)(13)			2
76 BID/BRE Vibrational levels not indicated.	EX	300	(1.35±0.22)(13)			2
77 LIL/RIC v≤13. Fast-flow reactor.	EX	150-300	(1.57±0.24)(14)	0	758±144	2
78 KOL Vibrational levels not indicated. Fast-flow reactor.	EX	300	(1.35±0.22)(13)			2
O + CS₂ → SO + CS (a) → S + COS (b) → S₂ + CO (c)						
Oxygen atom + Carbon disulfide						
71 TAK k _a . Step (a) is followed by the very fast reaction tion: O + CS → CO + S.	EX	298	(1.42±0.20)(12)			2
75 WEI/TIM k _a .	EX	218-293	(1.66±0.23)(13)	0	644±35	2
74 SLA/GIL k _b /(k _a + k _b + k _c).	RL	302	9.3(-2)			2/2
77 GRA/GUT k _b /(k _a + k _b + k _c). Within the given T range, the ratio decreases from 0.098±0.004 to 0.081±0.007.	RL	249-500	(9.8±0.4)(-2)			2/2
77 GRA/GUT k _a + k _b + k _c . Non-linear Arrhenius behaviour. Within the given T range, k increases from 1.75x10 ¹² to 6.75x10 ¹² cm ₃ mol ⁻¹ s ⁻¹ .	EX	249-500	(1.75±0.12)(12)			2 1.3
74 SLA/GIL k _a + k _b + k _c .	EX	302	2.41(12)			2
79 HSU/SHA k _c . Flash-photolysis. Laser Resonance- absorption.	EX	298	(3.5±0.5)(10)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + COS → CO + SO (a) → CO ₂ + S (b)						
Oxygen atom + Carbon oxide sulfide						
71 KRE k _a .	RN	300-523	9.82(12)	0	2265	2
71 KRE/SIM k _a .	EX	300-523	9.78(12)	0	2265	2
72 BRE/MIL k _a . Fast-flow technique with EPR detection. P(Total) = 0.45 torr.	EX	297	(7.2±0.4)(9)			2
74 KLE/STI k _a .	EX	263-502	(9.94±0.78)(12)	0	2167±28	2
75 WEI/TIM k _a .	EX	239-404	(1.2±0.2)(13)	0	2149±35	2
78 YOS/SAI k _a . Fast flow-reactor. Microwave Spectroscopy. P = 0.13 torr.	EX	298	(7.1±0.7)(9)			2
80 ROB/SMI k _a . Pulsed laser photolysis of O ₃ in excess N ₂ and in presence of COS. P(Total) = 100 torr.	EX	296	(1.02±0.12)(10)			2
82 TOP k _b . Oxidation of COS behind reflected shock- waves. Time-of-flight Mass-spectrometry. P = (1.3-2.7) atm.	EX	1200-1900	5.01(13)	0	5527±636	2
81 KRU/WAG ¹⁾ k _a + k _b . M = Ar. n = 0 assumed.	EX	298-1900	7.5(13)	0	2755	2
81 KRU/WAG ¹⁾ k _a + k _b . M = Ar. Recommended k. The preexponential factor expressed as: A(T/298) ¹ .	RE	298-1900	7.45(12)	1.0	2057	2
¹⁾ Measurement of O atoms concentration profiles by Resonance-absorption spectroscopy in shock- tube. O atoms generated by decomposition of N ₂ O in Ar.						
O(¹ D) + COS → CO + SO						
Oxygen atom + Carbon oxide sulfide						
75 GAU/SNE k _{ref} : O(¹ D) + O ₂ → O + O ₂ (¹ Σ _g ⁺)	RL	300	(4.1±0.6)			2/2
75 GAU/SNE	RN	300	1.81(14)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O + CH_3SH \rightarrow OH + CH_3S$ (a)						
$\rightarrow H + CH_3S(O)$ (b)						
$\rightarrow HS(O) + CH_3$ (c)						
$\rightarrow CH_3S(O)H$ (d)						
Oxygen atom + Methanethiol						
78 KIR/VET k_a . Initial step. Fast-flow reactor. Supersonic molecular beam. Mass-spectrometry.	EX	300-661	(8.5±1.0)(12)	0	625±36	2
78 SLA/BAI k_a . Fast flow-reactor. Photoionization Mass-spectrometer. Non-linear Arrhenius behaviour. k increases to $2.59 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 495 K.	EX	254	1.14(12)			2
81 NIP/SIN k_a . Phase-shift. O generated by Hg-photosensitized decomposition of N_2O . Gas-chromatography. 1) The Arrhenius plot for the rate constant of this reaction is sharply curved, but it can be fitted to the empirical expression: $k = (m) + (n)$, where $(m) = (9.15 \pm 1.02) \times 10^{11}$ and $(n) = (3.85 \pm 2.40) \times 10^{13} \exp(-1673 \pm 322/T)$	EX	298-560	1)	1)	1)	2
76 SLA/GRA $k_b + k_c + k_d$.	EX	300	1.14(12)			2
$O + CN(v=n) \rightarrow CO + N(^4S)$ (a)						
$\rightarrow CO^{\dagger} + N(^4S)$ (b)						
$\rightarrow CO^{\dagger} + N(^2D)$ (c)						
Oxygen atom + Cyanogen						
72 SCH/WOL2 k_a . Unreported T assumed to be 298 K. k unchanged from $v=0$ to $v=5$, but decreasing to $6.0 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at $v=6$.	EX	298	8.0(12)			2
73 SCH/SCH1 k_a . $n = 0$ to 6.	EX	298	1.26(13)			2
73 SCH/SCH1 k_a . $n = 7$.	EX	298	6.31(13)			2
75 ALB/HOY k_a . T-independent within the T-range 275-387 K. $v = 0$.	EX	298	(1.2±0.4)(13)			2
77 SCH/WOL $k_b + k_c$.	EX	295	(1.1±0.3)(13)			2
78 SCH/WOL $k_b + k_c$. Resonance-absorption Spectroscopy.	EX	298	(1.0±0.4)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units factor	k err. factor
O + NCO → NO + CO							
Oxygen atom + Cyanato							
74 SCH/SCH	EX	298	8.91(12)				2
O + HCN → H + OCN (a) → OH + CN (b)							
Oxygen atom + Hydrocyanic acid							
82 ROT/LOE2 ¹⁾ k _a .	EX	1500-2600	7.23(13)	0	7460		2
82 ROT/LOE2 ¹⁾ (k _a + k _b)/k _a .	RL	1500-2600	1.6				2/2
82 ROT/LOE2 ¹⁾ k _b .	RN	1500-2600	4.34(13)	0	7460		2
¹⁾ M = Ar. Reaction of O atoms with HCN behind reflected shock-waves. O atoms generated by fast N ₂ O decomposition. Atomic-resonance Absorption-spectrometry. Same data reported in 80 ROT/LOE. [HCN] = (0.62-4.92) × 10 ¹⁵ molec.cm ⁻³ . P = 1275 torr.							
O + CH₃NH₂ → products							
Oxygen atom + Methanamine							
74 KIR/MER Flow reactor. Ultrasonic molecular beam. Mass-spectrometer.	EX	300-450	(2.7±0.3)(12)	0	770±36		2
78 ATK/PIT1 ¹⁾	EX	298-440	5.43(12)	0	830±101		2
78 ATK/PIT1 ¹⁾	EX	298	(3.40±0.34)(11)				2
¹⁾ Flash-photolysis. NO ₂ chemilumcence.							
O + CH₃ONO → OH + HCHO + NO							
Oxygen atom + Nitrous acid methyl ester							
75 DAV/THR	EX	300-410	1.4(13)	0	2622±241		2
O + CH₃NO₂ → CH₃O + NO₂ (a) → OH + CH₂NO₂ (b)							
Oxygen atom + Methane, nitro-							
75 CAM/GOO1 k _a + k _b .	EX	295	(1.9±0.3)(9)				2
O + C₂O → CO + CO							
Oxygen atom + Carbon oxide (C ₂ O)							
72 SHA/MAS	EX	300	5.72(13)				2 1.61

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + CH₂=C → CO + CH(A²Δ)						
Oxygen atom + Ethynyl						
82 GRE/HOM2 Reaction of the CH ₂ =C/O/H system, diluted in N ₂ /He. O atoms generated by reacting N with NO. Discharge-flow. Resonance-fluorescence. P = 2 torr.	EX	298	≈7.0(11)			2
O + CH₂=CH → CO + CH₂ (a)						
→ H + CH ₂ =C=O → CH ₂ =C=O (b)						
→ C=C=O + H ₂ (c)						
Oxygen atom + Ethyne						
73 GAE/GLA k _a . Upper-limit k.	RN	300	≤1.3(11)			2
73 PEE/MAH2 k _a .	EX	1200-1700	5.2(13)	0	1862	2
77 VAN/VAN k _a .	ES	700-1430	6.7(13)	0	2013	2
81 LOE/ROT k _a . Oxydation of CH ₂ =CH behind shock-waves. Atomic Resonance-absorption Spectroscopy.	EX	1500-2570	1.20(14)	0	3300	2
81 TSU/HAS k _a . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ mixtures, behind reflected shock-waves.	ES	1200-1800	2.00(13)	0	1563	2
82 ROT/LOE2 k _a . M = Ar. Reaction of O atoms with CH ₂ =CH behind reflected shock-waves. O atoms generated by fast N ₂ O decomposition. Atomic-Resonance Absorption-spectroscopy. P = 1275 torr. [CH ₂ =CH] = (2.46-3.69)×10 ¹⁵ molec.cm ⁻³ . [N ₂ O] = (0.22-2.16)×10 ¹⁵ molec.cm ⁻³ .	EX	1500-2600	1.20(14)	0	3300	2
73 GAE/GLA k _b . M = N ₂ . Limiting high-pressure, upper-limit k.	RN	300	≤1.7(11)			2
81 ALE/ARU k _b . Recording of O and H atoms under jet conditions. Resonance-fluorescence.	EX	298-608	(9.03±0.24)(12)	0	2285±217	2
81 LOE/ROT k _b . M = Ar. Oxidation of Ethyne behind shock-waves. Atomic-Resonance Absorption-Spectroscopy.	EX	1500-2570	4.34(14)	0	6100	2
81 TSU/HAS k _b . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ mixtures, behind reflected shock-waves.	ES	1200-1800	2.00(13)	0	1564	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

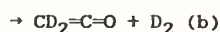
Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 ROT/LOE2 k _b . M = Ar. Reaction of O atoms with CH≡CH behind reflected shock-waves. O atoms generated by fast N ₂ O decomposition. Atomic-resonance Absorption- spectrometry. P = 1275 torr. [CH≡CH] = (2.46-3.69)x10 ¹⁵ molec.cm ⁻³ . [N ₂ O] = (0.22-2.16)x10 ¹⁵ molec.cm ⁻³ .	EX	1500-2600	4.34(14)	0	6100	2	
71 STU/NIK2 ¹⁾	EX	300	7.89(10)			2	1.1
77 WES/DEH ¹⁾	EX	297	(7.2±0.2)(10)			2	
76 HAN/MYE ¹⁾ Discharge-flow . Time-of-flight Mass-spectro- meter.	EX	300-408	1.38(13)	0	1500	2	1.23
81 ALE/ARU ¹⁾ Recording of O and H atoms under jet conditions. Resonance-fluorescence.	EX	298-608	(1.81±0.18)(13)	0	1624±108	2	
¹⁾ k _a + k _b .							
73 JON/BAY2 k _a + k _b + k _c .	EX	296	(9.7±1.5)(10)			2	
O + CD≡CD → CO + CD₂ (a)							
→ D + CD=C=O → CD₂=C=O (b)							
Oxygen atom + Ethyne-d₂							
71 STU/NIK2 k _a + k _b .	EX	300	7.89(10)			2	1.1
O + CH₂=CH₂ → HCHO + CH₂ (a)							
→ CHO + CH₃ (b)							
→ CH₂=C=O + H₂ (c)							
→  (d)							
Oxygen atom + Ethene							
73 PEE/MAH2 k _a .	ES	1200-1600	2.5(13)	0	2516	2	
73 GAE/GLA ¹⁾	ES	300	≈7.0(11)			2	
73 HUI ¹⁾	EX	232-500	(3.26±0.18)(12)	0	569±16	2	
73 KUR/HUI ¹⁾	EX	298	4.79(11)			2	1.1
73 PEE/MAH2 ¹⁾	EX	1200-1700	2.26(13)	0	1359	2	
76 MAN/BRA ¹⁾ Flash-photolysis. Resonance-fluorescence. P(Total) = 5 torr.	EX	298	(4.51±0.24)(11)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 SUG/ISH1 ¹⁾ Pulse-radiolysis. Resonance-absorption. Predominant path. P = (50-950) torr.	EX	296	(6.02±1.20)(11)			2
¹⁾ k _b .						
74 PRU/SLA k _b /(k _b + k _c).	RL	300	9.5(-1)			2/2
82 NIC/RAV ²⁾	EX	298	(4.32±0.44)(11)			2
82 NIC/RAV ²⁾ Arrhenius plot is linear below 500 K, but exhibits a curvature above 500 K. Measured k's above 500 K are: 552 K: (1.6±0.2)(12); 695 K: (2.4±0.3)(12); 708 K: (2.3±0.2)(12); 736 K: (2.7±0.3)(12); 811 K: (3.0±0.4)(12); 835 K: (3.5±0.9)(12); 944 K: (4.2±1.2)(12).	EX	298-500	(7.35±3.73)(12)	0	870±190	2
²⁾ k _b + k _c . Flash-photolysis. Resonance- fluorescence. O atoms generated by Flash-photolysis of O ₂ . [CH ₂ =CH ₂] = (0.01-2.0)×10 ¹⁵ molec.cm ⁻³ . [O] ~ (2-4)×10 ¹⁰ molec.cm ⁻³ . P(Ar) = 100 torr.						
82 TEM/WAG2 ³⁾ k _b /(k _a + k _b + k _c + k _d). P = 0.75 torr.	RL	298	3.5(-1)			2/2
82 TEM/WAG2 ³⁾ k _b /(k _a + k _b + k _c + k _d). P = 3.0 torr.	RL	298	6.0(-1)			2/2
³⁾ Reaction of O with Ethene in a isothermal dis- charge-flow reactor, in He. LMR-spectrometry.						
74 PRU/SLA k _c .	EX	300	(2.29±0.57)(10)			2
73 GAE/GLA k _d . Limiting high-pressure k. M = N ₂ .	ES	300	≈7.0(11)			2
71 ATK/CVE k _a + k _b + k _c + k _d .	EX	298	(3.0±2.0)(11)			2
71 STU/NIK2 k _a + k _b + k _c + k _d .	EX	300	3.79(1)			2 1.15
72 ATK/CVE k _a + k _b + k _c + k _d .	EX	298-473	8.1(12)	0	976±50	2
72 ATK/CVE k _a + k _b + k _c + k _d .	EX	298	(3.0±0.2)(11)			2
72 DAV/HUI k _a + k _b + k _c + k _d .	EX	232-500	(3.26±0.18)(12)	0	569±16	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
72 STU/NIK3 $k_a + k_b + k_c + k_d$.	EX	298	(3.76±0.38)(11)			2
74 ATK/PIT1 $k_a + k_b + k_c + k_d$.	EX	300-392	3.37(12)	0	639±101	2
74 ATK/PIT2 $k_a + k_b + k_c + k_d$.	EX	301	(4.0±0.4)(11)			2
74 FUR/ATK $k_a + k_b + k_c + k_d$.	EX	298	(4.3±0.5)(11)			2
74 MCC ($k_a + k_b + k_c + k_d$)/ k_{ref} . k_{ref} : $O + (CH_3)_2C=CH_2 \rightarrow$ products.	RL	298	(4.2±1.0)(-2)			2/2
74 SLA/PRU $k_a + k_b + k_c + k_d$.	EX	300	4.64(12)			2
76 SIN/CVE $k_a + k_b + k_c + k_d$.	EX	298-480	(6.89±0.89)(12)	0	845±47	2
77 ATK/PIT1 $k_a + k_b + k_c + k_d$.	EX	298-439	5.56(12)	0	742±101	2 1.1
77 ATK/PIT1 $k_a + k_b + k_c + k_d$.	EX	298	(4.58±0.46)(11)			2

Oxygen atom + Ethene-d₄

73 KUR/HUI k_a .	EX	298	4.93(11)			2 1.1
72 STU/NIK3 $k_a + k_b$.	EX	298	(3.37±0.34)(11)			2
82 NIC/RAV ¹⁾ $k_a + k_b$.	EX	298	(4.48±0.38)(11)			2
82 NIC/RAV ¹⁾ $k_a + k_b$. Arrhenius plot is linear below 500 K, but exhibits a curvature above 500 K. Measured k's above 500 K are: 523 K: (1.5±0.1)(+12); 595 K: (1.8±0.2)(+12); 708 K: (2.3±0.2)(+12); 811 K: (2.6±0.3)(+12).	EX	298-500	(7.35±3.73)(12)	0	870±190	2

¹⁾ Flash-photolysis. Resonance-fluorescence, O
atoms generated by Flash-photolysis of O₂.

$$[CD_2=CD_2] = (0.01-2.0) \times 10^{15} \text{ molec.cm}^{-3}.$$

$$[O] \sim (2-4) \times 10^{10} \text{ molec.cm}^{-3}.$$

$$P(Ar) = 100 \text{ torr.}$$

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O(^1D) + CH_2=CH_2 \rightarrow \text{products}$						
Oxygen atom + Ethene						
79 KAJ/FUE N ₂ O photolysis. Gas-chromatography. P(Total) = 200 torr. k _{ref} : $O(^1D) + N_2O \rightarrow N_2 + O_2$	RL	298	(1.8±0.4)			2/2
$O + CH_3CH_2 \rightarrow H + CH_3CHO$ (a) $\rightarrow CH_3 + HCHO$ (b)						
Oxygen atom + Ethyl						
79 HOY/SIE3 k _a /k _b . Nozzle reactor. Mass-spectrometry.	RL	298	(5.0±1.0)			2/2
$O + CH_3CH_3 \rightarrow HCHO + H_2 + CH_2$ (a) $\rightarrow OH + CH_3CH_2$ (b)						
Oxygen atom + Ethane						
71 AVR/KOL1 k _a .	EX	313-523	(1.23±0.60)(12)	0	2164±352	2
71 AVR/KOL1 ¹⁾	EX	313-523	(2.29±1.14)(13)	0	3775±352	2
71 PAP/ASH ¹⁾	EX	300-365	2.75(13)	0	3271±126	2 1.48
80 TAN/KLE ¹⁾	EX	416-1048	(1.12±0.04)(14)	0	3949±36	2
Reaction of O atom with Ethane in a Quartz tube. Flash-photolysis. Discharge-flow. Resonance-fluorescence. [O] = (1.0-3.0) atoms.cm ⁻³ . Pressure-independent k.						
82 CAY/PEE ¹⁾	EX	600-1030	(1.9±0.8)(14)	0	4806±159	2
Discharge flow. Molecular beam sampling. Mass-spectrometry.						
¹⁾ k _b .						
$O(^1D) + CH_3CH_3 \rightarrow OH + CH_3CH_2$						
Oxygen atom + Ethane						
74 MIC/PAR k _{ref} : $O(^1D) + (CH_3)_4C \rightarrow \text{products}$.	RL	300	(5.12±0.05)(-1)			2/2
76 FLE/HUS	EX	300	(4.39±0.48)(14)			2
81 PRA/PAU Photolysis of O ₂ /CH ₃ CH ₃ mixtures diluted in He. P(O ₂) >15 torr. P(He) = 600 torr. k _{ref} = $O(^1D) + O_2 \rightarrow O(^3P) + O_2$	RL	298	(1.24±0.06)(1)			2/2
$O + CH=C=O \rightarrow CO + CO + H$						
Oxygen atom + Ethenyl, 2-oxo-						
73 JON/BAY1	EX	298	(1.2±0.3)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O + CH₂=C=O → products							
Oxygen atom + Ethenone (Ketene)							
73 JON/BAY2	EX	296	(1.7±0.4)(11)			2	
74 MAC/THR2	EX	293	(3.4±0.3)(11)			2	
The predominant step is: O + CH ₂ =C=O → CHO + CHO							
75 GAF/ATK1 ¹⁾	RL	296	(2.4±0.2)(-2)			2/2	
k _{ref} : O + CH=CHCH ₂ CH ₂ CH ₂ → products.							
75 GAF/ATK1 ¹⁾	RN	296	(2.78±0.35)(11)			2	
Determined relative to the reaction:							
O + CH=CHCH ₂ CH ₂ CH ₂ → products.							
¹⁾ Competitive technique. Static high-vacuum technique. O atoms generated by Hg-photosensitized dissociation of N ₂ O. Gas-chromatography.							
O + CH₃CHO → OH + CH₃CO (a)							
→ OH + CH ₂ CHO (b)							
→ HCHO + H ₂ + CO (c)							
→ CO ₂ + H ₂ + CH ₂ (d)							
Oxygen atom + Acetaldehyde							
71 AVR/KOL2 ¹⁾	EX	373-428	1.60(10)	0	604	2	
74 MAC/THR1 ¹⁾	EX	300	(2.88±0.3)(11)			2	
77 MIC/LEE ¹⁾	EX	298	(2.95±0.30)(11)			2	
Discharge-flow. Resonance-fluorescence.							
77 SIN/IRW ¹⁾	ES	298-472	(7.00±1.40)(12)	0	977±77	2	
Phase-shift.							
81 MOR1 ¹⁾	EX	298	(2.9±0.4)(11)			2	
Discharge-flow. Time-of-flight. Mass-spectrometry. Gas-chromatography.							
¹⁾ k _a .							
77 SIN/IRW	EX	298-472	(7.21±1.49)(12)	0	986±77	2	
k _a + k _b . Phase-shift.							
71 AVR/KOL2	EX	373-428	4.28(12)	0	2919	2	
k _b .							
71 AVR/KOL2	EX	373-428	8.79(10)	0	1158	2	
k _c + k _d .							
O +  → OH + 							
Oxygen atom + Oxirane (Ethylene epoxide)							
78 BOG/HAN ¹⁾	EX	298-691	1.91(12)	0	2642±75	2	1.20
Suggested realistic error limits are: a factor of 3 at 300 K and a factor of 1.5 AT 700 K.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 BOG/HAN ¹⁾	RL	482-691	(9.0±2.0)(1)	0	-735±116	2/2	
$k_{\text{ref}}: \text{O} + \text{D}_2\text{C}_2\text{D}_2 \rightarrow \text{OD} + \text{D}_2\text{C}_2\text{D}_2^{\cdot}$							
¹⁾ Discharge-flow. Mass-spectrometry. Photometry.							
$\text{O} + \text{HC(O)OCH}_3 \rightarrow \text{OH} + \text{C(O)OCH}_3$							
Oxygen atom + Formic acid methyl ester (Methyl formate)							
81 MOR1	EX	298	(5.6±1.1)(9)			2	
Discharge-flow. Mass-spectrometry.							
82 FAU/HOY	EX	298	(6.4±2.5)(8)			2	
Reaction of O with HCOOCH ₃ in a flow-system.							
P = (4-8) torr. [O] = (2.2-6.6) × 10 ¹⁴ molec.cm ⁻³ .							
$\text{O} + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{OH} + \text{CH}_3\text{CHOH} \quad (\text{a})$							
$\rightarrow \text{OH} + \text{CH}_2\text{CH}_2\text{OH} \quad (\text{b})$							
$\rightarrow \text{OH} + \text{CH}_3\text{CH}_2\text{O} \quad (\text{c})$							
$\rightarrow \text{HCHO} + \text{CH}_2 + \text{H}_2\text{O} \quad (\text{d})$							
$\rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CHO} \quad (\text{e})$							
Oxygen atom + Ethanol							
76 OWE/ROS	EX	301-439	4.17(8)	0	758±204	2	1.12
k _a . Flow reactor.							
71 AVR/KOL2 ¹⁾	EX	343-413	1.87(13)	0	2944	2	
81 WAS ¹⁾	EX	298	(1.02±0.18)(11)			2	
Fast-flow reactor. Mass-spectrometry. O atoms generated by a He/O ₂ mixture, by a microwave-discharge.							
P(Total) = (3.73-3.88) torr.							
¹⁾ k _a + k _b + k _c .							
71 AVR/KOL2	EX	343-523	3.43(11)	0	1334	2	
k _d .							
71 AVR/KOL2	EX	343-413	7.47(11)	0	1485	2	
k _e .							
$\text{O} + \text{CD}_3\text{CD}_2\text{OH} \rightarrow \text{OD} + \text{CD}_3\text{CDOH} \quad (\text{a})$							
$\rightarrow \text{OD} + \text{CD}_2\text{CD}_2\text{OH} \quad (\text{b})$							
$\rightarrow \text{OH} + \text{CD}_3\text{CD}_2\text{O} \quad (\text{c})$							
Oxygen atom + Ethan-d ₅ -ol							
81 WAS	EX	298	(6.62±2.41)(10)			2	
k _a + k _b + k _c . Fast-flow reactor. Photoionization Mass-spectrometry. O atoms generated in a He/O ₂ mixture, in a microwave-discharge.							
P(Total) = 3.73 mtorr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	E, B-B(ref)	k, A units	k err. factor
$O + (CH_3)_2O \rightarrow OH + CH_2OCH_3$							
Oxygen atom + Methane, oxybis- (Dimethyl ether)							
72 LEF/MEA	EX	217-366	(5.0±1.0)(12)	0	1434±101	2	
82 FAU/HOY	EX	298	(2.3±0.7)(10)			2	
Reaction of O with HCOOCH ₃ in a flow-system.							
[O] = (2.2-6.0)×10 ¹⁴ molec.cm ⁻³ .							
P = (41-101) torr.							
$O + \triangle \rightarrow SO + CH_2=CH_2$							
Oxygen atom + Thiirane (Ethylene episulfide)							
76 LEE/TIM	EX	298-478	(8.07±0.54)(12)	0	18±20	2	
$O + CH_3CH_2SH \rightarrow OH + CH_3CH_2S$ (a)							
→ HS(O) + CH ₃ CH ₂ (b)							
→ H + CH ₃ CH ₂ S(O) (c)							
→ CH ₃ CH ₂ S(O)H (d)							
Oxygen atom + Ethanethiol (Ethyl mercaptan)							
78 KIR/VET	EX	304-421	(5.75±0.3)(12)	0	391±18	2	
k _a . Initial step in a suggested mechanism.							
Supersonic molecular beam.							
Fast flow-reactor.							
Mass-spectrometry.							
78 SLA/BAI	EX	257	1.93(12)			2	
k _a . Fast flow.							
Photoionization Mass-spectrometry.							
Non-linear Arrhenius behaviour.							
k increasing to 3.19×10 ¹² cm ³ mol ⁻¹ s ⁻¹							
at 495 K.							
81 NIP/SIN	EX	298-560	¹⁾	¹⁾	¹⁾	2	
k _a . Phase-shift technique. $\dot{O}$ atoms generated by							
Hg-photosensitized decomposition of N ₂ O.							
Gas-chromatography.							
¹⁾ The Arrhenius plot for k of this reaction is							
sharply curved, but it can be fitted to the							
empirical expression:							
k = (m) + (n),							
where: (m) = (1.37±0.07)×10 ¹² and							
(n) = (8.73±4.46)×10 ¹³ exp(-2075±268/T)							
76 SLA/GRA	EX	300	1.69(12)			2	
k _b + k _c + k _d .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + (CH₃)₂S → CH₃S(O) + CH₃ (a)						
→ CH₃O + CH₃S (b)						
Oxygen atom + Methane, thiobis- (Dimethyl sulfide)						
78 SLA/BAI	EX	252	3.79(13)			2
k _a . Fast flow. Photoionization Mass-spectrometry. Possible non-linear Arrhenius behaviour.						
k decreasing to:						
2.17x10 ¹³ cm ³ mol ⁻¹ s ⁻¹ at 493 K.						
80 LEE/TAN1	EX	272-472	(7.71±0.72)(12)	0	-404±30	2
k _a . Fast-flow. Resonance-fluorescence.						
81 NIP/SIN	EX	298-560	(6.69±0.72)(12)	0	-460±41	2
k _a . Phase-shift.						
O atoms formed by Hg-photosensitized decomposition of N ₂ O. Gas-chromatography.						
74 CAD/WIC ¹⁾	EX	300	3.3(11)			2
76 LEE/TIM ¹⁾	EX	268-424	(8.55±0.42)(12)	0	-366±16	2
76 SLA/GRA ¹⁾	EX	300	3.79(13)			2
¹⁾ k _a + k _b .						
O + CH₃SSCH₃ → products						
Oxygen atom + Disulfide, dimethyl-						
80 LEE/TAN2	EX	270-329	(1.28±0.13)(14)	0	0	2
Discharge fast-flow. Resonance-fluorescence.						
P = (0.52-2.60) torr.						
81 NIP/SIN	EX	298-560	(2.62±0.42)(13)	0	-251±61	2
Phase-shift. O atoms formed by Hg-photosensitized decomposition of N ₂ O. Gas-chromatography.						
O + CH₃CN → OCN + CH₃						
Oxygen atom + Acetonitrile						
77 BON/TIM	EX	383-500	(4.38±1.05)(11)	0	2401±101	2
77 BON/TIM ¹⁾	RL	383	(1.2±0.3)			2/2
77 BON/TIM ¹⁾	RL	423	(1.5±0.6)			2/2
¹⁾ k _{ref} : O + CD ₃ CN → OCN + CD ₃						
O + CH₃CH₂NH₂ → products						
Oxygen atom + Ethanamine						
74 KIR/MER	EX	300-450	(3.9±0.3)(12)	0	529±24	2
Flow reactor. Ultrasonic molecular beam.						
Mass-spectrometer.						
78 ATK/PIT1 ¹⁾	EX	298-440	6.81(12)	0	642±101	2
78 ATK/PIT1 ¹⁾	EX	299	(8.01±0.84)(11)			2
¹⁾ Flash-photolysis. NO ₂ chemiluminescence.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + (CH₃)₂NH → products						
Oxygen atom + Methanamine, N-methyl-						
74 KIR/MER Ultrasonic molecular beam. Mass-spectrometer. Flow reactor.	EX	300	3.2(12)			2
78 ATK/PIT1 ¹⁾	EX	298-440	9.15(12)	0	277±101	2
78 ATK/PIT1 ¹⁾	EX	298	(3.69±0.37)(12)			2
¹⁾ NO ₂ chemiluminescence. Flash-photolysis.						
O + CH₃CH₂ONO → OH + CH₃CHO + NO						
Oxygen atom + Nitrous acid ethyl ester						
75 DAV/THR	EX	300-410	2.6(13)	0	2442±241	2
O + O=C=C=C=O → CO + CO + CO						
Oxygen atom + 1,2-Propadiene-1,3-dione						
74 PIL/WAG	EX	250-450	(1.0±0.2)(13)	0	1100±170	2
O(¹D) + O=C=C=C=O → CO + CO + CO						
Oxygen atom + 1,2-Propadiene-1,3-dione						
73 HEI/HUS2	EX	300	(2.41±0.24)(14)			2
O + CH₃C≡CH → CO + CH₃CH (a) → H + [C₃H₃O] (b)						
Oxygen atom + 1-Propyne						
73 HER k _a . Assumed to pass through a vibrationally excited intermediate: 2-Methyloxirene.	EX	275-360	1.6(13)	0	1010	2
74 HER/WAG k _a . Isothermal flow-system. P = (5-40) torr.	EX	290-360	1.3(13)	0	1007±201	2
81 ALE/DUB ¹⁾ k _b .	EX	295-545	(3.61±1.20)(12)	0	1323±217	2
81 ALE/DUB ¹⁾ k _{overall} .	EX	295-545	(8.43±2.42)(12)	0	866±108	2
¹⁾ Recording of O and H atoms under jet conditions. Resonance-fluorescence.						
75 ARR/COX k _{overall} .	EX	298-600	(1.39±0.36)(13)	0	981±352	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$O + CH_2=C=CH_2 \rightarrow CO + CH_2=CH_2$ (a)							
$\rightarrow H + [C_3H_3O]$ (b)							
Oxygen atom + 1,2-Propadiene (Allene)							
72 HER/WAG	EX	275-375	7.8(12)	0	805	2	1.3
k_a .							
73 HER	EX	275-360	7.8(12)	0	806	2	
k_a . Assumed to pass through a vibrationally excited intermediate:							
Methyleneoxirane.							
74 HAV ¹⁾	RL	298	6.6(-1)			2/2	
k_{ref} : $O + CH_3CH_2CH=CH_2 \rightarrow$ products.							
74 HAV ¹⁾	RL	298	1.97(-1)			2/2	
k_{ref} : $O + (CH_3)_2C=CH_2 \rightarrow$ products.							
¹⁾ k_a/k_{ref} . Two vibrationally excited precursors are suggested:							
Methyleneoxirane, or Cyclopropanone.							
80 ALE/ARU2	EX	295-860	6.63(12)	0	1535±151	2	
k_b . Resonance-fluorescence.							
77 ATK/PIT2 ²⁾	EX	297-439	1.23(13)	0	883±101	2	1.1
77 ATK/PIT2 ²⁾	EX	298	(6.44±0.66)(11)			2	
79 NIP/SIN ²⁾	EX	297-574	(1.80±0.25)(13)	0	941±54	2	
Modulated, Hg-sensitized N ₂ O decomposition.							
Phase-shift.							
80 ALE/ARU2 ²⁾	EX	295-860	1.02(13)	0	956±101	2	
Resonance-fluorescence.							
²⁾ $k_{overall}$.							
$O + CH_3CH=CH_2 \rightarrow$  (a)							
$\rightarrow OH + CH_2CH=CH_2$ (b)							
$\rightarrow CH_3CHO + CH_2$ (c)							
$\rightarrow HCHO + H_2 + CH_2=C$ (d)							
Oxygen atom + 1-Propene							
72 KUR1	EX	201-424	(2.51±0.20)(12)	0	38±22	2	
k_a , or possibly k_b .							
73 GAE/GLA	RN	300	≈2.9(12)			2	
k_a . M = N ₂ . Estimated k.							
73 HER	EX	275-360	4.2(12)	0	253	2	
k_a .							
71 AVR/KOL1	EX	373-583	7.23(12)	0	2718	2	
k_b .							
71 AVR/KOL1	EX	361-483	5.06(10)	0	755	2	
k_c .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
71 AVR/KOL1 k _d .	EX	361-483	5.42(11)	0	1258	2
71 ATK/CVE ¹)	EX	298	(1.18±0.06)(12)			2
71 STU/NIK2 ¹)	EX	300	2.17(12)			2 1.1
72 ATK/CVE ¹)	EX	298-473	6.7(12)	0	518±50	2
72 ATK/CVE ¹)	EX	298	(1.18±0.06)(12)			2
73 GAE/GLA ¹)	RN	300	≈2.7(12)			2
74 ATK/PIT1 ¹)	EX	300-392	2.08(12)	0	0±151	2
74 ATK/PIT2 ¹)	EX	300	(2.01±0.22)(12)			2
74 FUR/ATK ¹)	EX	298	(2.02±0.17)(12)			2
75 GAF/ATK1 ¹)	RN	296	2.10(12)			2
76 SIN/CVE ¹)	EX	298-480	(7.58±0.42)(12)	0	363±20	2
77 ATK/PIT1 ¹)	EX	298-439	6.32(12)	0	259±101	2 1.1
77 ATK/PIT1 ¹)	EX	299	(2.69±0.27)(12)			2
77 MIC/LEE ¹)	EX	298	(2.38±0.25)(12)			2
Resonance-fluorescence. Discharge-flow.						
80 SUG/ISH1 ¹)	EX	296	(2.83±0.18)(12)			2
Resonance-absorption. Pulse-radiolysis. P = (50-950) torr.						
82 BIE/HAR ¹)	EX	298	(2.65±0.36)(12)			2
Photoionization Mass-spectrometry. Discharge-flow system. P(Total) ~ 2 torr.						
¹) k _{overall} .						
74 MCC k _{overall} /k _{ref} . k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.	RL	298	(2.0±0.5)(-1)			2/2
75 GAF/ATK1 k _{overall} /k _{ref} . Competitive technique. Static system. O-atoms generated by Hg-photosensitized dissociation of N ₂ O. Gas-chromatography. k _{ref} : O + CH=CHCH ₂ CH ₂ CH ₂ → products.	RL	296	(1.81±0.10)(-1)			2/2
O(¹ D) + CH ₃ CH=CH ₂ → products						
Oxygen atom + 1-Propene						
79 KAJ/FUE N ₂ O photolysis. Gas-chromatography. k _{ref} : O(¹ D) + N ₂ O → N ₂ + O ₂ P(Total) = 200 torr.	RL	298	(5.0±1.0)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{O} + \triangle \rightarrow \text{OH} + \triangle^{\bullet}$						
Oxygen atom + Cyclopropane						
76 LEE	EX	298-478	(3.31±0.42)(12)	0	3120±60	2
$\text{O} + \text{CH}_3\text{CH}_2\text{CH}_2 \rightarrow \text{H} + \text{CH}_3\text{CH}_2\text{CHO} \quad (\text{a})$ $\rightarrow \text{HCHO} + \text{CH}_3\text{CH}_2 \quad (\text{b})$						
Oxygen atom + Propyl						
79 HOY/SIE3	RL	298	(6.0±1.5)			2/2
k_a/k_b . Low pressure nozzle reactor. Mass-spectrometry.						
$\text{O} + (\text{CH}_3)_2\text{CH} \rightarrow \text{H} + (\text{CH}_3)_2\text{CO} \quad (\text{a})$ $\rightarrow \text{CH}_3 + \text{CH}_3\text{CHO} \quad (\text{b})$						
Oxygen atom + Ethyl, 1-methyl- (Isopropyl)						
79 HOY/SIE3	RL	298	(1.0±0.2)			2/2
k_a/k_b . Low pressure nozzle reactor. Mass-spectrometry.						
$\text{O} + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{OH} + (\text{CH}_3)_2\text{CH} \quad (\text{a})$ $\rightarrow \text{OH} + \text{CH}_3\text{CH}_2\text{CH}_2 \quad (\text{b})$						
Oxygen atom + Propane						
75 HAR/BUR	EX	329	(3.9±0.7)(10)			2
$k_a + k_b$.						
81 JEW/HOL	EX	306	(4.7±0.8)(9)			2
$k_a + k_b$. Discharge-flow reactor. O atoms produced by reacting N with NO. Gas-chromatography.						
$\text{O}(^1\text{D}) + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{OH} + (\text{CH}_3)_2\text{CH} \quad (\text{a})$ $\rightarrow \text{OH} + \text{CH}_3\text{CH}_2\text{CH}_2 \quad (\text{b})$						
Oxygen atom + Propane						
75 GAU/SNE ¹⁾	RN	300	4.82(14)			2
76 FLE/HUS ¹⁾	EX	300	(5.72±0.60)(14)			2
¹⁾ $k_a + k_b$.						
74 MIC/PAR	RL	300	(6.52±0.27)(-1)			2/2
$(k_a + k_b)/k_{\text{ref}}$. k_{ref} : $\text{O}(^1\text{D}) + (\text{CH}_3)_4\text{C} \rightarrow \text{products}$.						
75 GAU/SNE	RL	300	(1.08±0.20)(1)			2/2
$(k_a + k_b)/k_{\text{ref}}$. k_{ref} : $\text{O}(^1\text{D}) + \text{O}_2 \rightarrow \text{O} + \text{O}_2(^1\Sigma_g^+)$						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 PRA/PAU ($k_a + k_b$)/ k_{ref} . Photolysis of O_2 /Propane mix- tures in He. $P(O_2) > 15$ torr. $P(He) = 600$ torr. $k_{ref} = O(^1D) + O_2 \rightarrow O(^3P) + O_2$	RL	298	(1.34 ± 0.04)(1)			2/2
$O + CH_2=CHCHO \rightarrow$ products						
Oxygen atom + 2-Propenal (Acrolein)						
72 CAD/LIN	EX	300-480	(4.7 ± 1.6)(12)	0	1007 ± 151	2
75 GAF/ATK1	RL	296	(2.0 ± 0.2)(-2)			2/2
$k_{ref}: O + $  $\rightarrow$ products.						
75 GAF/ATK1	RN	296	(2.3 ± 0.23)(11)			2
75 GAF/ATK2	RL	296	(2.0 ± 0.2)(-2)			2/2
75 GAF/ATK2 ¹⁾	RN	296-423	1.4(13)	0	1208 ± 136	2
75 GAF/ATK2 ¹⁾	RN	296	(2.32 ± 0.23)(11)			2
¹⁾ Competitive technique. Static system. O atoms generated by Hg-photosensitized dissociation of N_2O . Gas-chromatography. k determined relative to the reaction:						
$O + $  $\rightarrow$ products,						
and placed on an absolute basis by using the k expression from the literature, for the reaction: $O + CH_3CH=CH_2 \rightarrow$ products. Supersedes 75 GAF/ATK1.						
$O + CH_2=CHOCH_3 \rightarrow$ products						
Oxygen atom + Ethene, methoxy-						
77 ATK/PIT2	EX	297-439	3.81(12)	0	-38 ± 101	2 1.1
77 ATK/PIT2	EX	297	(4.30 ± 0.43)(12)			2
$O + CH_3CH_2CHO \rightarrow OH + CH_3CH_2C$ (a)						
$\rightarrow OH + CH_3CHCHO$ (b)						
$\rightarrow OH + CH_2CH_2CHO$ (c)						
Oxygen atom + Propanal						
72 CAD/LIN $k_a + k_b + k_c$.	EX	300-480	(8.5 ± 2.8)(13)	0	1912 ± 252	2
77 SIN/IRW ¹⁾ k_a .	ES	298-472	(5.67 ± 0.51)(12)	0	777 ± 31	2
77 SIN/IRW ¹⁾ $k_a + k_b + k_c$.	EX	298-472	(7.78 ± 0.75)(12)	0	869 ± 33	2
¹⁾ Phase-shift technique.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + (CH₃)₂CO → OH + CH₃COCH₂							
Oxygen atom + 2-Propanone							
72 AZA/GYU	EX	873	8.43(10)			2	
76 AMB/BRA	EX	298-621	4.27(12)	0	2863±84	2	1.26
Discharge-flow. ESR detection.							
76 LEE	EX	298-478	(1.86±0.37)(12)	0	2536±101	2	
77 LEE/TIM	EX	298-478	(1.9±0.4)(12)	0	2536±91	2	
82 FAU/HOY	EX	298	(6.8±2.9)(8)			2	
Reaction of O with HCOOCH ₃ in a flow-system.							
[O] = (3.3-4.0)×10 ¹⁴ molec.cm ⁻³ .							
P = (5-10) torr.							
O + HC(O)OCH₂CH₃ → OH + C(O)OCH₂CH₃							
Oxygen atom + Formic acid ethyl ester (Ethyl formate)							
82 FAU/HOY	EX	298	(1.0±0.4)(9)			2	
Reaction of O with HCOOCH ₃ in a flow-system.							
[O] = (2.2-7.2)×10 ¹⁴ molec.cm ⁻³ .							
P = (5-17) torr.							
O + CH₃C(O)OCH₃ → OH + CH₃C(O)OCH₂ (a)							
→ OH + CH₂C(O)OCH₃ (b)							
Oxygen atom + Acetic acid methyl ester (Methyl acetate)							
82 FAU/HOY	EX	298	(4.9±2.0)(8)			2	
k _a + k _b . Reaction of O with HCOOCH ₃							
in a flow-system. P = (4-8) torr.							
[O] = (3.3-7.8)×10 ¹⁴ molec.cm ⁻³ .							
O + CH₃CH₂CH₂OH → OH + CH₃CH₂CHOH (a)							
→ OH + CH₃CH₂CH₂O (b)							
Oxygen atom + 1-Propanol							
79 AYU/ROS	EX	463-308	7.92(11)	0	1500±165	2	1.10
k _a + k _b . Initial steps in a suggested mechanism.							
Fast-flow system. Microwave-discharge.							
Gas-chromatography. Mass-spectrometry.							
O + (CH₃)₂CHOH → OH + (CH₃)₂COH (a)							
→ OH + (CH₃)₂CHO (b)							
Oxygen atom + 2-Propanol							
79 AYU/ROS	EX	306-428	3.19(11)	0	1100±143	2	1.07
k _a + k _b . Initial steps in a suggested mechanism.							
Gast-flow system. Microwave-discharge.							
Gas-chromatography. Mass-spectrometry.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + CH₃CH₂CH₂SH → OH + CH₃CH₂CH₂S						
Oxygen atom + 1-Propanethiol (Propyl mercaptan)						
78 KIR/VET Initial step in a suggested mechanism. Supersonic molecular beam. Fast-flow reactor. Mass-spectrometry.	EX	303-421	(8.33±0.54)(12)	0	494±22	2
O + (CH₃)₃N → products						
Oxygen atom + Methanamine, N,N-dimethyl-						
74 KIR/MER Ultrasonic molecular beam. Mass-spectrometer. Flow reactor.	EX	300	9.4(12)			2
78 ATK/PIT1 ¹⁾	EX	298-440	6.50(12)	0	209±101	2
78 ATK/PIT1 ¹⁾	EX	298	(1.33±0.13)(13)			2
¹⁾ NO ₂ chemiluminescence. Flash-photolysis.						
O + CH≡CC≡CH → products						
Oxygen atom + 1,3-Butadiyne						
73 JON/BAY2	EX	296	(1.6±0.5)(12)			2
75 HOM/SCH	EX	297-343	8.0(13)	0	1230	2
O + CH₂=CHC≡CH → products						
Oxygen atom + 1-Buten-3-yne						
75 HOM/SCH	EX	295	(2.95±0.10)(12)			2
O + CH₃CH₂C≡CH → CO + CH₃CH=CH₂						
Oxygen atom + 1-Butyne						
75 HER/WAG1	EX	290-357	1.7(13)	0	800	2
77 UMS/LIN CO laser resonant absorption. NO ₂ Flash-photolysis.	EX	298	5.0(11)			2
O + CH₃C≡CCH₃ → CO + CH₃CH=CH₂						
Oxygen atom + 2-Butyne						
75 HER/WAG2	ES	290-360	6.0(13)	0	900	2
77 UMS/LIN CO laser resonant absorption. NO ₂ Flash-photolysis.	EX	298	1.6(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + CH₃CH=C=CH₂ → products						
Oxygen atom + 1,2-Butadiene						
74 HAV k _{ref} : O + CH ₃ CH ₂ CH=CH ₂ → products.	RL	298	1.39			2/2
74 HAV k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.	RL	298	4.3(-1)			2/2
O + CH₂=CHCH=CH₂ → products						
Oxygen atom + 1,3-Butadiene						
74 MCC k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.	RL	298	(9.6±3.5)(-1)			2/2
77 ATK/PIT2	EX	297-439	1.36(13)	0	53±101	2 1.1
77 ATK/PIT2	EX	297	(1.17±0.11)(13)			2
79 NIP/SIN Hg-sensitized N ₂ O decomposition. Phase-shift.	EX	299-488	(1.25±0.13)(13)	0	0	2
80 SUG/ISH1 Pulse-radiolysis. Resonance-absorption. P = (50-950) torr.	EX	296	(1.20±0.12)(13)			2
O + CH₃CH₂CH=CH₂ → products						
Oxygen atom + 1-Butene						
71 ATK/CVE	EX	298	(1.55±0.12)(12)			2
71 HUI/HER	EX	259-493	(8.79±0.90)(12)	0	382±30	2
72 ATK/CVE	EX	298-473	6.1(12)	0	408±50	2
72 ATK/CVE	EX	298	(1.55±0.12)(12)			2
72 HUI/HER2 Flash-photolysis. Resonance-fluorescence. 1) Curved Arrhenius plot. Authors give two additive empirical exponential terms: k _a = (2.23±1.08)×10 ¹² exp(-25±105/T) and k _b = (9.64±5.42)×10 ¹² exp(-991±216/T) in units of cm ³ mol ⁻¹ s ⁻¹ . They ascribe k _a O-atom addition and k _b to H-abstraction.	EX	190-491	¹⁾ ¹⁾		¹⁾	2 1.6
74 FUR/ATK	EX	298	(2.40±0.32)(12)			2
74 HAV k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.	RL	298	2.3(-1)			2/2
74 MCC k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.	RL	298	(1.8±0.7)(-1)			2/2
76 SIN/CVE	EX	298-480	(7.21±0.44)(12)	0	333±23	2
77 ATK/PIT1	EX	298-439	8.37(12)	0	335±101	2 1.1
77 ATK/PIT1	EX	299	(2.73±0.28)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
80 SUG/ISH1 Pulse-radiolysis. Resonance-absorption. P = (50-950) torr.	EX	296	(2.83±0.30)(12)			2	
O + cis-CH₃CH=CHCH₃ → products							
Oxygen atom + 2-Butene, (Z)-							
73 DAV/HUI	EX	268-443	(5.84±0.58)(12)	0	-161±32	2	
74 FUR/ATK	EX	298	(9.00±1.76)(12)			2	
74 HAV k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.	RL	298	9.5(-1)			2/2	
74 MCC k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.	RL	298	(7.9±2.5)(-1)			2/2	
76 SIN/CVE	EX	298-480	(6.68±0.23)(12)	0	-135±13	2	
77 ATK/PIT1	EX	298-439	7.29(12)	0	-118±101	2	1.1
77 ATK/PIT1	EX	299	(1.09±0.11)(13)			2	
80 SUG/ISH1 Pulse-radiolysis. Resonance-absorption. P = (50-950) torr.	EX	296	(1.20±0.18)(13)			2	
O(¹D) + cis-CH₃CH=CHCH₃ → products							
Oxygen atom + 2-Butene, (Z)-							
79 KAJ/FUE N ₂ O photolysis. Gas-chromatography. k _{ref} : O(¹ D) + N ₂ O → N ₂ + O ₂ P(Total) = 200 torr.	RL	298	(7.2±1.5)			2/2	
O + trans-CH₃CH=CHCH₃ → products							
Oxygen atom + 2-Butene, (E)-							
74 MCC k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.	RL	298	(1.25±0.35)			2/2	
77 ATK/PIT1	EX	298-439	1.36(13)	0	-10±101	2	1.1
77 ATK/PIT1	EX	299	(1.42±0.14)(13)			2	
80 SUG/ISH1 Pulse-radiolysis. Resonance-absorption. P = (50-950) torr.	EX	296	(1.39±0.18)(13)			2	
O(¹D) + trans-CH₃CH=CHCH₃ → products							
Oxygen atom + 2-Butene, (E)-							
79 KAJ/FUE N ₂ O photolysis. Gas-chromatography. k _{ref} : O(¹ D) + N ₂ O → N ₂ + O ₂ P(Total) = 200 torr.	RL	298	(4.9±1.0)			2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + (CH₃)₂C=CH₂ → products						
Oxygen atom + 1-Propene, 2-methyl-						
71 ATK/CVE	EX	298	(6.2±1.5)(12)			2
72 ATK/CVE	EX	298-473	6.3(12)	0	0±201	2
72 ATK/CVE	EX	298	(6.2±1.5)(12)			2
74 FUR/ATK	EX	298	(9.85±1.34)(12)			2
76 SIN/CVE	EX	298-480	(8.74±0.53)(12)	0	-51±22	2
77 ATK/PIT1	EX	298-439	1.06(13)	0	43±101	2 1.1
77 ATK/PIT1	EX	299	(9.22±0.11)(12)			2
80 SUG/ISH1	EX	296	(1.02±0.12)(13)			2
Pulse-radiolysis. Resonance-absorption.						
P = (50-950) torr.						
O(¹D) + (CH₃)C=CH₂ → products						
Oxygen atom + 1-Propene, 2-methyl-						
79 KAJ/FUE	RL	298	(3.7±1.0)			2/2
N ₂ O photolysis. Gas-chromatography.						
P(Total) = 200 torr.						
k _{ref} : O(¹ D) + N ₂ O → N ₂ + O ₂						
O + (CH₃)₂C=CHD → products						
Oxygen atom + 1-Propene-1-d ₁ , 2-methyl-						
76 HAV/HUN	RL	298-302	(1.03±0.01)	0	0	2/2
k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.						
O + (CH₃)₂C=CD₂ → products						
Oxygen atom + 1-Propene, 1,1-d ₂ , 2-methyl-						
76 HAV/HUN	RL	298-302	(1.05±0.01)	0	0	2/2
k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.						
O + (CH₃)₂CHCH₂ → H + (CH₃)₂CHCHO (a)						
→ HCHO + (CH ₃) ₂ CH (b)						
Oxygen atom + Propyl, 2-methyl-						
79 HOY/SIE3	RL	298	(7.0±2.0)			2/2
k _a /k _b . Low pressure nozzle reactor.						
O + (CH₃)₃C → OH + (CH₃)₂C=CH₂ (a)						
→ CH ₃ + (CH ₃) ₂ CO (b)						
Oxygen atom + Ethyl, 1,1-dimethyl-						
80 WAS/BAY	RN	297	(5.24±1.14)(14)			2
k _a + k _b . Fast-flow reactor system. Photoionization Mass-spectrometer. k measurements by Stern-Volmer plots. P(Total) = (1.8-5.7) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O + CH₃CH₂CH₂CH₃ → OH + CH₃CH₂CH₂CH₂ (a)							
→ OH + CH₃CH₂CHCH₃ (b)							
Oxygen atom + Butane							
71 PAP/ASH ¹⁾	EX	300-365	1.66(13)	0	2280±121	2	1.45
74 ATK/PIT2 ¹⁾	EX	301	(1.88±0.20)(10)			2	
77 ATK/PER1 ¹⁾	EX	298-439	1.51(13)	0	2099±151	2	
77 ATK/PER1 ¹⁾	EX	298	(1.32±0.24)(10)			2	
¹⁾ k _a + k _b .							
O(¹D) + CH₃CH₂CH₂CH₃ → products							
Oxygen atom + Butane							
74 MIC/PAR	RL	300	(8.63±0.33)(-1)			2/2	
k _{ref} : O(¹ D) + (CH ₃) ₄ C → products.							
O + (CH₃)₃CH → OH + (CH₃)₃C (a)							
→ OH + (CH₃)₂CHCH₂ (b)							
Oxygen atom + Propane, 2-methyl-							
80 WAS/BAY	EX	297	(6.02±1.20)(10)			2	
k _a + k _b . Fast-flow. Photoionization Mass-spectrometer. P(Total) = (1.8-5.7) torr.							
82 JEW/HOL	EX	307	(7.9±1.4)(10)			2	
k _a + k _b . Reaction of O with Isobutane. Discharge-flow. Gas-chromatography. P = (2-4) torr.							
O + CH₃CH=CHCHO → products							
Oxygen atom + 2-Butenal (Crotonaldehyde)							
74 CAD/WIC	EX	~300	2.0(13)	0	1158	2	
74 CAD/WIC	EX	300	5.0(11)			2	
75 GAF/ATK1	RL	296	(4.4±0.5)(-2)			2/2	
k _{ref} : O +  → products.							
75 GAF/ATK1	RN	296	(5.10±0.58)(11)			2	
75 GAF/ATK2	RL	296	(4.4±0.5)(-2)			2/2	
75 GAF/ATK2 ¹⁾	RN	296-423	1.5(13)	0	996±65	2	
75 GAF/ATK2 ¹⁾	RN	296	(5.10±0.58)(11)			2	
¹⁾ Competitive technique. Static system. O atoms generated by Hg-photosensitized dissociation of N ₂ O. Gas-chromatography. k determined relative to the reaction:							
O +  → products,							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
and placed on an absolute basis by using the k expression from the literature, for the reaction: $O + CH_3CH=CH_2 \rightarrow \text{products}$. Supersedes 75 GAF/ATK1.						
$O + CH_3CH_2CH_2CHO \rightarrow OH + CH_3CH_2CH_2CO$ (a)						
$\rightarrow OH + CH_3CH_2CHCHO$ (b)						
$\rightarrow OH + CH_3CHCH_2CHO$ (c)						
$\rightarrow OH + CH_2CH_2CH_2CHO$ (d)						
Oxygen atom + Butanal						
74 JAF/WAN ¹⁾	ES	298	1.5(11)			2
77 SIN/IRW ¹⁾	ES	298-472	(6.23±0.13)(12)	0	719±8	2
Phase-shift.						
¹⁾ k _a .						
77 SIN/IRW	EX	298-472	(9.99±0.56)(12)	0	857±20	2
k _a + k _b + k _c + k _d .						
Phase-shift.						
$O + (CH_3)_2CHCHO \rightarrow OH + (CH_3)_2CHCO$ (a)						
$\rightarrow OH + (CH_3)_2CCHO$ (b)						
$\rightarrow OH + CH_2CH(CH_3)CHO$ (c)						
Oxygen atom + Propanal, 2-methyl-						
77 SIN/IRW	ES	298-472	(7.18±0.87)(12)	0	700±43	2
k _a .						
Phase-shift.						
77 SIN/IRW	EX	298-472	(7.92±1.02)(12)	0	727±46	2
k _a + k _b + k _c .						
Phase-shift.						
$O + (CH_3CH_2)_2O \rightarrow OH + CH_3CHOCH_2CH_3$ (a)						
$\rightarrow OH + CH_2CH_2OCH_2CH_3$ (b)						
Oxygen atom + Ethane, 1,1'-oxybis-						
82 FAU/HOY	EX	298	(6.7±3.5)(10)			2
k _a + k _b . Reaction of O with HCOOCH ₃ in a flow-system. P = (12-50) torr. [O] = (3.3-4.0)×10 ¹⁴ molec.cm ⁻³ .						
$O + \text{Thiophene} \rightarrow \text{products}$						
Oxygen atom + Thiophene						
81 LEE/TAN	EX	262-448	(2.01±0.20)(13)	0	569±30	2
Discharge-flow system. Resonance-fluorescence. [O] ₀ = (0.5-1.0)×10 ¹¹ atoms.cm ⁻³ .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + CH₃CH₂CH₂CH₂SH → OH + CH₃CH₂CH₂CH₂S						
Oxygen atom + 1-Butanethiol (Butyl mercaptan)						
78 KIR/VET Initial step in a suggested mechanism. Supersonic molecular beam. Fast flow-reactor. Mass-spectrometry.	EX	306-419	(5.78±0.33)(12)	0	321±19	2
O + NCC≡CCN → NCCO + CCN						
Oxygen atom + 2-Butynedinitrile						
72 HAN/OBE1 Predominant first step. Discharge-flow reactor. Time-of-flight Mass-spectrometry. P(Total) = 137 torr.	EX	298	(6.63±1.81)(8)			2
76 HAN/MYE Predominant first step. Discharge-flow reactor. Time-of-flight Mass-spectrotry. P = (0.73-1.10) torr.	EX	300-408	7.94(12)	0	2768±554	2 5.01
O + CH₃CH₂CH₂C≡CH → CO[†] + CH₃CH₂CH₂CH:						
Oxygen atom + 1-Pentyne						
80 SHA/BUR Flash-photolysis. CO laser Resonance-absorption.	EX	293	(4.9±0.6)(11)			2
O + (CH₃)₂C=C=CH₂ → products						
Oxygen atom + 1,2-Butadiene, 3-methyl-						
74 HAV k _{ref} : O + (CH ₃) ₂ C=CHCH ₃ → products.	RL	298	7.6(-1)			2/2
O +  → products						
Oxygen atom + Cyclopentene						
75 GAF/ATK2 Competitive technique. Static system. O atoms generated by Hg-photosensitized dissociation of N ₂ O. Gas-chromatography. k placed on an absolute basis by using the k expression from the literature, for the reaction: O + CH ₃ CH=CH ₂ → products. Supersedes 75 GAF/ATK1.	RN	296-423	5.6(12)	0	-216±40	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

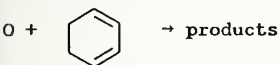
Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O +  → products							
Oxygen atom + Spiropentane							
72 HUI/HER3 Discharge-flow. Mass-spectrometry.	EX	337-652	3.98(13)	0	2890±100	2	1.26
O + CH ₃ CH ₂ CH ₂ CH=CH ₂ → products							
Oxygen atom + 1-Pentene							
82 BIE/HAR Photoionization Mass-spectrometry. Discharge-flow. P(Total) ~ 2 torr.	EX	298	(2.83±0.30)(12)			2	
O + (CH ₃) ₂ CHCH=CH ₂ → products							
Oxygen atom + 1-Butene, 3-methyl-							
74 MCC k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.	RL	298	(2.2±0.5)(-1)			2/2	1.2
76 SIN/CVE	EX	298-480	(6.02±0.44)(12)	0	266±26	2	
O + (CH ₃) ₂ C=CHCH ₃ → products							
Oxygen atom + 2-Butene, 2-methyl-							
74 FUR/ATK	EX	298	(3.11±0.30)(13)			2	
78 ATK/PIT2 NO ₂ chemiluminescence. Flash-photolysis.	EX	299-441	1.51(13)	0	-191±101	2	
80 SUG/ISH1 Resonance-absorption. Pulse-radiolysis. P = (50-950) torr.	EX	296	(3.31±0.30)(13)			2	
O(¹ D) + (CH ₃) ₂ C=CHCH ₃ → products							
Oxygen atom + 2-Butene, 2-methyl-							
79 KAJ/FUE N ₂ O photolysis. Gas-chromatography. P(Total) = 200 torr. k _{ref} : O(¹ D) + N ₂ O → N ₂ + O ₂	RL	298	(8.9±2.0)			2/2	
O +  → products							
Oxygen atom + Cyclopentane							
72 HUI/HER3 Discharge-flow. Mass-spectrometry.	EX	337-652	1.26(14)	0	2210±100	2	1.23

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O + (CH_3)_3CCH_2 \rightarrow H + (CH_3)_3CCHO$ (a)						
$\rightarrow HCHO + (CH_3)_3C$ (b)						
Oxygen atom + Propyl, 2,2-dimethyl-						
79 HOY/SIE1	RN	300	3.3(13)			2
$k_a + k_b$.						
Low pressure nozzle reactor.						
Mass-spectrometry.						
P = (0.01-0.2) torr.						
$O(^1D) + CH_3CH_2CH_2CH_2CH_3 \rightarrow$ products						
Oxygen atom + Pentane						
74 MIC/PAR	RL	300	(9.88±0.32)(-1)			2/2
$k_{ref}: O(^1D) + (CH_3)_4C \rightarrow$ products.						
$O + (CH_3)_4C \rightarrow OH + (CH_3)_3CCH_2$						
Oxygen atom + Propane, 2,2-dimethyl- (Neopentane)						
82 MIC/KEI	EX	415-922	(9.15±1.69)(13)	0	3595±99	2
Reaction of O atoms with Neopentane						
in Ar/N ₂ buffer gas.						
Discharge-flow. Resonance-fluorescence.						
O atoms generated by the photodecomposition of O ₂ .						
P(Neopentane) = (44.3-215) mtorr.						
P(Total) = (30-100) torr.						
P(O ₂) = (0.40-6.0) torr.						
$O(^1D) + (CH_3)_4C \rightarrow$ products						
Oxygen atom + Propane, 2,2-dimethyl- (Neopentane)						
71 SCO/CVE	RL	296	(4.29±0.25)			2/2
$k_{ref}: O(^1D) + N_2O \rightarrow O_2 + N_2$ (a)						
$\rightarrow NO + NO$ (b)						
75 GAU/SNE	RL	300	(1.4±0.2)(1)			2/2
$k_{ref}: O(^1D) + O_2 \rightarrow O + O_2(^1\Sigma_g^+)$						
75 GAU/SNE	RN	300	6.26(14)			2
76 FLE/HUS	EX	300	(7.41±0.78)(14)			2
$O + CH_3CH_2CH_2CH_2CH_2SH \rightarrow OOH + CH_3CH_2CH_2CH_2CH_2S$						
Oxygen atom + 1-Pentanethiol (Pentyl mercaptan)						
78 KIR/VET	EX	302-409	(6.18±0.35)(12)	0	328±19	2
Initial strep in a suggested mechanism.						
Supersonic molecular beam.						
Fast flow-reactor.						
Mass-spectrometry.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

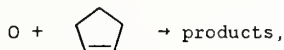
Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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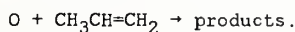
Oxygen atom + 1,3-Cyclohexadiene

75 GAF/ATK2 ¹⁾	RN	296-423	5.1(12)	0	-664±91	2
75 GAF/ATK2 ¹⁾	RN	296	(5.03±0.23)(13)			2

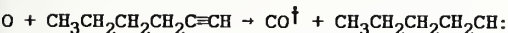
¹⁾ Competitive technique. Static system. O atoms generated by Hg-photosensitized dissociation of N₂O. Gas-chromatography. k determined relative to the reaction:



and placed on an absolute basis by using the k expression from the literature, for the reaction:



Supersedes 75 GAF/ATK1.



Oxygen atom + 1-Hexyne

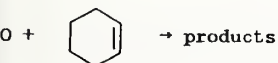
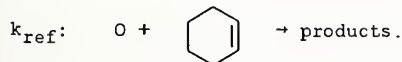
80 SHA/BUR	EX	293	(3.6±0.4)(11)			2
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Flash-photolysis. CO laser Resonance-absorption.



Oxygen atom + 2,3-pentadiene, 2-methyl-

74 HAV	RL	298	3.03			2/2
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Oxygen atom + Cyclohexene

82 WAS/TAK	EX	298	(1.20±0.03)(13)			2
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Reaction of Cyclohexene with O atoms in a fast flow-reactor.

O atoms generated by a microwave-discharge in a He/O₂ mixture.

Mass-spectrometry.

P(Cyclohexene) = (0.004-0.012) mtorr.

[O₂]₀ = (0.266-0.560) mtorr.

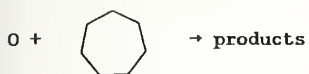
P(Total) = 3.7 torr.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O + (CH₃)₂C=C(CH₃)₂ → products							
Oxygen atom + 2-Butene, 2,3-dimethyl-							
74 FUR/ATK	EX	298	(4.44±0.41)(13)				2
73 DAV/HUI	EX	298-355	(3.36±0.64)(12)	0	-790±60		2
75 SIN/FUR	EX	298-481	(1.24±0.12)(13)	0	-390±38		2
O +  → OH + 							
Oxygen atom + Cyclohexane → Hydroxyl + Cyclohexyl							
75 KIM/TIM	EX	344-513	(3.2±0.6)(14)	0	2214±201		2
Reaction of Oxygen atom with Cyclohexane in an ESR-flow apparatus. Mass-spectrometry. [Cyclohexane] = (1.8-6.0)10 ¹³ molec.cm ⁻³ . P = (0.33-0.94) torr.							
82 WAS/TAK	EX	298	(5.84±0.36)(10)				2
Reaction of Cyclohexane with O atoms in a fast-flow reactor. O atoms generated by a microwave-discharge in a He/O ₂ mixture. Mass-spectrometry. P(Cyclohexane) = (0.010-0.028) mtorr. P(Total) = (3.8-3.9) torr. [O ₂] ₀ = (13.7-16.1) mtorr.							
72 HUI/HER3	EX	337-652	2.23(14)	0	2350±100		2 1.23
k _b . Discharge-flow. Mass-spectrometry.							
O +  → products							
Oxygen atom + Cyclohexene, 1-methyl-							
75 GAF/ATK2 ¹⁾	RN	296-423	5.3(12)	0	-669±111		2
75 GAF/ATK2 ¹⁾	RN	296	(4.89±0.20)(13)				2
¹⁾ Competitive technique. Static system. O atoms generated by Hg-photosensitized dissociation of N ₂ O. Gas-chromatography. k determined relative to the reaction:							
O +  → products,							
and placed on an absolute basis by using the k expression from the literature, for the reaction:							
O + CH ₃ CH=CH ₂ → products.							
Supersedes 75 GAF/ATK1.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

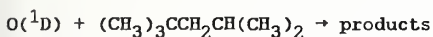
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
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Oxygen atom + Cycloheptane

72 HUI/HER3 EX 337-652 2.88(14) 0 2230±100 2 1.3

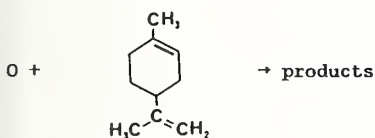
Discharge-flow. Mass-spectrometry.



Oxygen atom + Pentane, 2,2,4-trimethyl-

74 MIC/FAR RL 300 (1.257±0.041) 2/2

k_{ref}: O(¹D) + (CH₃)₄C → products.



Oxygen atom + Cyclohexene, 1-methyl-

4-(1-methylethenyl)-, (R)-

(d-Limonene, or (+)-Limonene)

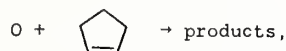
75 GAF/ATK2 ¹⁾ RN 296-423 1.1(14) 0 151±75 2

75 GAF/ATK2 ¹⁾ RN 296 (6.50±0.53)(13) 2

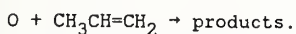
¹⁾ Competitive technique. Static system.

O atoms generated by Hg-photosensitized dissociation of N₂O. Gas-chromatography.

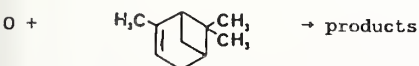
k determined relative to the reaction:



and placed on an absolute basis by using the k expression from the literature, for the reaction:



Supersedes 75 GAF/ATK1.

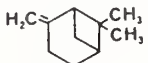


Oxygen atom + Bicyclo[3.1.1]hept-2-ene,

2,6,6-trimethyl- (α-Pinene)

75 GAF/ATK2 ¹⁾ RN 296-423 7.5(13) 0 458±70 2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 GAF/ATK2 ¹⁾ ¹⁾ Competitive technique. Static system. O-atoms generated by Hg-photosensitized dissociation of N ₂ O. k determined relative to the reaction: $\text{O} + \text{Cyclopentadiene} \rightarrow \text{products},$ and placed on an absolute basis by using the k expression from the literature, for the reaction: $\text{O} + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{products}.$ Supersedes 75 GAF/ATK1.	RN	296	(1.60±0.06)(13)			2
O +  → products						
Oxygen atom + Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene- (β-Pinene)						
75 GAF/ATK2 ¹⁾	RN	296-423	6.0(13)	0	413±70	2
75 GAF/ATK2 ¹⁾	RN	296	(1.51±0.06)(13)			2
¹⁾ Competitive technique. Static system. O atoms generated by Hg-photosensitized dissociation of N ₂ O. k determined relative to the reaction: $\text{O} + \text{Cyclopentadiene} \rightarrow \text{products},$ and placed on an absolute basis by using the k expression from the literature, for the reaction: $\text{O} + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{products}.$ Supersedes 75 GAF/ATK1.						
O ₂ (+ M) → O + O (+ M) Oxygen molecule						
71 BRE/BIR M = Kr. M-efficiencies relative to Kr are: 1.0(Kr), ~1.6(Xe), ~1.0(Ar), ~9.0(O ₂).	EX	4000-8500	7.87(13)	0	52743	2
O ₂ (¹ A _g) + O ₃ → O ₂ + O ₂ + O Oxygen molecule + Ozone						
71 FIN/SNE	EX	283-321	2.74(13)	0	2828±181	2
72 BEC/GRO	EX	296-360	3.61(13)	0	2854±143	2
72 HUS/KIR1 Upper-limit k.	EX	300	<6.02(9)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
73 COL/HUS	EX	300	(2.65±0.78)(9)			2
74 SNE	EX	298	(1.39±0.30)(13)			2
80 ARN/COM UV-photolysis of Ozone.	EX	298	(3.07±0.30)(9)			2
74 KUR/BRA $k_{\text{ref}}: \text{O}_2(^1\Delta_g) + \text{O}_3^{\dagger} \rightarrow \text{O}_2 + \text{O}_2 + \text{O}$ $\text{O}_3^{\dagger}$ formed by absorption of CO_2 laser radiation.	RL	300	(2.63±0.91)(-2)			2/2
$\text{O}_2(^1\Sigma_g^+) + \text{O}_3 \rightarrow \text{O}_2 + \text{O}_2 + \text{O} \text{ (a)}$ $\quad \quad \quad \rightarrow \text{O}_2 + \text{O}_3 \text{ (b)}$						
Oxygen molecule + Ozone						
82 OGR/SWO $k_a + k_b$. Flash-photolysis of O_2/O_3 mixtures in a vacuum system. $P(\text{Total}) = 100 \text{ torr}$.	EX	298	(1.1±0.2)(13)			2
$\text{O}_2^{\dagger} + \text{O}_3 \rightarrow \text{O} + \text{O}_2 + \text{O}_2$						
Oxygen molecule + Ozone						
80 ARN/COM UV-photolysis of Ozone. O_2 is vibrationally excited, with $v \leq 30$.	EX	298	(1.69±0.18)(9)			2
$\text{O}_2 + \text{H}_2 \rightarrow \text{OH} + \text{OH} \text{ (a)}$ $\quad \quad \quad \rightarrow \text{HO}_2 + \text{H} \text{ (b)}$						
Oxygen molecule + Hydrogen molecule						
71 BEL/BRA k_a . Constant tube-area.	ES	1128-1152	2.10(12)	0	19628	2
71 BEL/BRA k_a . Varying tube-area.	ES	1128-1152	1.20(12)	0	19628	2
71 JAC/HOU k_a . Reaction behind incident shock-waves, in Ar. UV-Absorption-spectroscopy.	EX	1200-1800	1.7(13)	0	24233	2 3.0
75 AZA/ALE k_a .	EX	1076-1523	1.90(4)	0	21892±503	2 1.58
72 SKI/LIF k_b .	ES	1000-2500	3.0(13)	0	31706	2
79 HAC/PRE1 k_b . Isothermal flow-reactor. Laser Magnetic Resonance Spectrometry. $P(\text{Total}) = (130-800) \text{ Pa}$.	DE	298	2.9(-29)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O₂ + D₂ → OD + OD						
Oxygen molecule + Deuterium molecule						
75 AZA/ALE	EX	843	(1.02±0.24)(3)			2
75 AZA/ALE	EX	843	(7.83±3.01)(2)			2
k based on induction period.						
O₂(¹Δ_g) + SO₂ → O + SO₃						
Oxygen molecule + Sulfur dioxide						
76 DUM	EX	298	1.3(8)			2
O₂ + CO₂[*] → O₃ + CO						
Oxygen molecule + Carbon dioxide						
71 PRA/MAK	RL	293	(5.0±2.0)(2)			2/2
M = CO.						
Photolysis of O ₂ + CO mixture.						
P(CO) = (1-60) torr.						
P(O ₂) = 40 torr.						
k _{ref} : CO ₂ [*] + M → CO ₂ ^{**} + M.						
CO [*] formed by O(¹ D) + CO.						
O₂ + CH₄ → HO₂ + CH₃						
Oxygen molecule + Methane						
72 SKI/LIF	ES	1000-2500	8.00(13)	0	28183	2
78 SHA	DE	300-2500	7.56(11)	2.0	26153	2
The preexponential factor expressed as:						
A(T/298) ² .						
82 PAR	EX	1097	<9.53(5)			2
Reaction of CH ₄ with O ₂ in single-pulse shock-waves.						
Mass-spectrometry.						
Upper-limit k.						
O₂ + HCHO → HO₂ + CHO						
Oxygen molecule + Formaldehyde						
71 BAL/LAN	RN	713	1.3(1)			2
74 BAL/FUL2	EX	713-816	2.04(13)	0	19577±755	2
O₂ + HCHO[*] [or HC(:)OH] → [HC(:)OH.O₂]						
Oxygen molecule + Formaldehyde (or Methylene, hydroxy-)						
79 MOR/HEI	RL	296	(7.9±0.6)(6)			2/1
HCHO photolysis at 313 nm.						
k _{ref} :						
HCHO [*] [or HC(:)OH] → H + CHO						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$O_2 + CH_3O_2NO + CH_3O_2NO \rightarrow CH_3ONO_2 + CH_3ONO_2 + O_2$							
Oxygen molecule + Peroxynitrous acid methyl ester							
73 SPI/VIL Determined on the basis of a suggested mechanism.	ES	298	$\approx 3.79(13)$			3	
$O_2 + C_2O \rightarrow CO_2 + CO$							
Oxygen molecule + Carbon oxide (C_2O)							
80 DON/PIT Laser photodissociation of C_3O_2 at 266 nm. Dye-laser induced fluorescence.	EX	298	$(1.99 \pm 0.07)(11)$			2	
$O_2(a^1\Delta_g) + CH \equiv CH \rightarrow \text{products}$							
Oxygen molecule + Ethyne							
79 DAT/RAO Microwave discharge-flow system.	EX	298	$(1.03 \pm 0.08)(7)$			2	
$O_2 + CH_3CHO (+M) \rightarrow HO_2 + CH_3CO (+M)$							
Oxygen molecule + Acetaldehyde							
74 DIX/SKI1 ¹⁾	RN	336	6.8(-3)			2	
74 DIX/SKI1 ¹⁾	RN	345	7.4(-3)			2	
74 DIX/SKI1 ¹⁾	RN	393	6.15(-2)			2	
¹⁾ Surface/volume ratio = 0.6 cm^{-1} .							
74 DIX/SKI1 ²⁾	RN	345	2.9(-2)			2	
74 DIX/SKI1 ²⁾	RN	393	5.1(-1)			2	
¹⁾ Surface/volume ratio = 6.1 cm^{-1} .							
77 COL/NAE The preexponential factor expressed as: $A(T/298)^{0.5}$.	ES	1030-1115	3.45(14)	0.5	21238 $\pm$ 604	2	2.0
76 BRY/LEV M = O_3 .	EX	393-473	5.01(17)	0	7549 $\pm$ 856	3	7.08
$O_2 + CH_3CH_2CHO \rightarrow HO_2 + CH_3CH_2CO$							
Oxygen molecule + Propanal							
71 BAL/LAN	RN	713	7.6(1)			2	
74 DIX/SKI1	RN	337	3.4(-2)			2	
79 BAL/LEW1 Oxidation in an aged boric-acid-coated vessel.	EX	713	$(8.1 \pm 1.5)(1)$			2	
$O_2(a^1\Delta_g) + (CH_3)_2CO \rightarrow \text{products}$							
Oxygen molecule + 2-Propanone							
79 DAT/RAO Microwave discharge flow system.	EX	298	$(5.9 \pm 0.8)(6)$			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$O_2(a^1A_g) + CH_3CH_2CH=CH_2 \rightarrow$ products							
Oxygen molecule + 1-Butene							
79 DAT/RAO Microwave discharge-flow system.	EX	298	(1.11±0.05)(7)			2	
$O_2(a^1A_g) + \text{cis-}CH_3CH=CHCH_3 \rightarrow$ products							
Oxygen molecule + 2-Butene, (Z)-							
75 ASH/OGR	EX	300-500	1.26(11)	0	3256±141	2	1.38
79 DAT/RAO Microwave discharge-flow system.	EX	298	(1.42±0.05)(7)			2	
$O_2(a^1A_g) + \text{trans-}CH_3CH=CHCH_3 \rightarrow$ products							
Oxygen molecule + 2-Butene, (E)-							
75 ASH/OGR	EX	300-500	1.518(11)	0	3664±181	2	1.51
79 DAT/RAO Microwave discharge-flow system.	EX	298	(1.50±0.07)(7)			2	
$O_2(a^1A_g) + (CH_3)_2C=CH_2 \rightarrow$ products							
Oxygen molecule + 1-Propene, 2-methyl-							
79 DAT/RAO Microwave discharge-flow system.	EX	298	(2.02±0.02)(7)			2	
$O_2(a^1A_g) + CH_3CH_2CH_2CH_3 \rightarrow$ products							
Oxygen molecule + Butane							
79 DAT/RAO Microwave discharge-flow system.	EX	298	(1.05±0.40)(6)			2	
$O_2(a^1A_g) + CH_3C(O)OCH=CH_2 \rightarrow$ products							
Oxygen molecule + Acetic acid ethenyl ester (Vinyl acetate)							
79 DAT/RAO Microwave discharge-flow system.	EX	298	(8.2±0.9)(6)			2	
$O_2(a^1A_g) + CH_2=CHC(O)OCH_3 \rightarrow$ products							
Oxygen molecule + 2-Propenoic acid methyl ester							
79 DAT/RAO Microwave discharge-flow system.	EX	298	(1.27±0.02)(7)			2	
$O_2 + (CH_3)_2CHCHO \rightarrow HO_2 + (CH_3)_2CHCO$							
Oxygen molecule + Propanal, 2-methyl-							
79 BAL/CLE Aged boric-acid-coated vessel. P(Total) = 60 torr.	EX	713	(1.2±0.1)(2)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O_2(a^1\Delta_g) + CH_3C(O)OCH_2CH_3 \rightarrow \text{products}$ Oxygen molecule + Acetic acid ethyl ester (Ethyl acetate)						
79 DAT/RAO Microwave discharge flow system.	EX	298	(6.3±0.1)(6)			2
$O_2(^1\Delta_g) + $  $\rightarrow \text{products}$ Oxygen molecule + Cyclopentene						
75 ASH/OGR	EX	300-500	2.24(11)	0	3719±357	2 2.29
$O_2(^1\Delta_g) + CH_3CH=C(CH_3)_2 \rightarrow \text{products}$ Oxygen molecule + 2-Butene, 2-methyl-						
73 HUI/HER k_{ref} : $O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow \text{products.}$	RL	298	4.4(-2)			2/2
73 HUI/HER	RN	298	3.3(7)			2
75 ASH/OGR	EX	300-500	1.26(11)	0	2466±141	2 1.45
$O_2 + (CH_3)_2CHCH_2CH_3 \rightarrow HO_2 + (CH_3)_2CCH_2CH_3$ (a) $\rightarrow HO_2 + (CH_3)_2CHCHCH_3$ (b) Oxygen molecule + Butane, 2-methyl- (Isopentane)						
73 DEG/DEN $k_a + k_b$.	EX	410-439	1.5(15)	0	19124	2
$O_2(^1\Delta_g) + $  $\rightarrow \text{products}$ Oxygen molecule + Furan, 2-methyl-						
73 HUI/HER k_{ref} : $O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow \text{products.}$	RL	298	1.3			2/2
73 HUI/HER	RN	298	1.0(8)			2
$O_2(a^1\Delta_g) + CH_2=CHC(O)OCH_2CH_3 \rightarrow \text{products}$ Oxygen molecule + 2-Propenoic acid ethyl ester						
79 DAT/RAO Microwave discharge flow system.	EX	298	(1.54±0.11)(7)			2

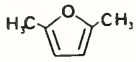
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O_2(^1\Delta_g) + CH_2=C(CH_3)C(O)OCH_3 \rightarrow$ products Oxygen molecule + 2-Propenoic acid, 2-methyl-, methyl ester						
79 DAT/RAO Microwave discharge flow system.	EX	298	(1.09±0.09)(7)			2
$O_2(^1\Delta_g) + $  $\rightarrow$ products						
Oxygen molecule + 1,3-Cyclohexadiene						
73 HUI/HER k_{ref} : $O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow$ products.	RL	298	9.0(-2)			2/2
73 HUI/HER	RN	298	6.8(7)			2
$O_2(^1\Delta_g) + $  $\rightarrow$ products						
Oxygen molecule + 1,4-Cyclohexadiene						
79 DAT/RAO Microwave discharge-flow system.	EX	298	(1.36±0.06)(7)			2
$O_2(^1\Delta_g) + $  $\rightarrow$ products						
Oxygen molecule + Cyclohexene						
75 ASH/OGF Lower-limit estimate.	ES	300-500	2.51(11)	0	>4127	2
79 DAT/RAO Microwave discharge-flow system.	EX	298	(4.7±1.5)(6)			2
$O_2(^1\Delta_g) + $  $\rightarrow$ products						
Oxygen molecule + Cyclopentene, 1-methyl-						
73 HUI/HER k_{ref} : $O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow$ products.	RL	298	1.5(-1)			2/2
73 HUI/HER	RN	298	1.1(7)			2
75 ASH/OGF	EX	300-500	2.51(11)	0	3010±141	2 1.45

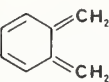
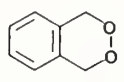
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$O_2(^1\Delta_g) + $  $ \rightarrow \text{products}$							
Oxygen molecule + Cyclobutene, 1,2-dimethyl-							
75 ASH/OGR	EX	300-500	2.75(11)	0	2011±91	2	1.29
$O_2(^1\Delta_g) + \text{trans-CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CHCH}_3 \rightarrow \text{products}$							
Oxygen molecule + 2-Pentene, 3-methyl-, (E)-							
73 HUI/HER	RL	298	~1.2(-2)			2/2	
Estimated ratio.							
$k_{\text{ref}}: O_2(^1\Delta_g) + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{products.}$							
73 HUI/HER	ES	298	~9.0(6)			2	
$O_2(^1\Delta_g) + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{products}$							
Oxygen molecule + 2-Butene, 2,3-dimethyl-							
72 ACK/PIT	EX	298	(4.9±0.3)(8)			2	
P > 3 torr.							
73 HUI/HER	EX	298	7.6(8)			2	
75 ASH/OGR	EX	300-500	1.32(11)	0	1626±75	2	1.23
76 DUM	EX	298	2.0(7)			2	
$O_2 + $  $ \rightarrow \text{HO}_2 + $ 							
Oxygen molecule + Cyclohexane							
75 SHA/DEN	EX	373-413	1.58(110)	0	12582±805	2	
$O_2(a^1\Delta_g) + $  $ \rightarrow \text{products}$							
Oxygen molecule + Cyclohexane							
79 DAT/RAO	EX	298	(1.08±0.30)(6)			2	
Microwave discharge-flow system.							
$O_2(a^1\Delta_g) + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{products}$							
Oxygen molecule + Hexane							
79 DAT/RAO	EX	298	(9.2±3.0)(5)			2	
Microwave discharge flow system.							

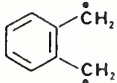
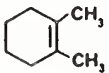
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{O}_2(^1\Delta_g) + $  $ \rightarrow \text{products}$							
Oxygen molecule + Furan, 2,5-dimethyl-							
73 HUI/HER	RL	298	1.9(1)				2/2
$k_{\text{ref}}: \text{O}_2(^1\Delta_g) + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{products}.$							
73 HUI/HER	RN	298	1.5(10)				2
$\text{O}_2(^1\Delta_g) + (\text{CH}_3)_2\text{CHCH}_2\text{OCH}=\text{CH}_2 \rightarrow \text{products}$							
Oxygen molecule + Propane, 1-(ethenyloxy)-2-methyl-							
79 DAT/RAO	EX	298	(1.17±0.12)(7)				2
Microwave discharge-flow system.							
$\text{O}_2(^1\Delta_g) + \text{CH}_3\text{C}(\text{O})\text{CH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{products}$							
Oxygen molecule + 2-Pentanone, 4-methyl-							
79 DAT/RAO	EX	298	(4.9±0.9)(6)				2
Microwave discharge-flow system.							
$\text{O}_2(^1\Delta_g) + (\text{CH}_3)_2\text{C}=\text{CHN}(\text{CH}_3)_2 \rightarrow \text{products}$							
Oxygen molecule + 1-Propen-1-amine, N,N,2-trimethyl-							
73 HUI/HER	RL	298	2.0(1)				2/2
$k_{\text{ref}}: \text{O}_2(^1\Delta_g) + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{products}.$							
73 HUI/HER	RN	298	1.5(10)				2
$\text{O}_2(^1\Delta_g) + $  $ \rightarrow \text{products}$							
Oxygen molecule + Cyclohexene, 1-methyl-							
75 ASH/OGF	EX	300-500	2.40(11)	0	3785±151	2	1.41
$\text{O}_2(^1\Delta_g) + $  $ \rightarrow \text{products}$							
Oxygen molecule + Cyclopentene, 1,2-dimethyl-							
73 HUI/HER	RL	298	4.0(-1)				2/2
$k_{\text{ref}}: \text{O}_2(^1\Delta_g) + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{products}.$							
73 HUI/HER	RN	298	3.0(8)				2
75 ASH/OGF	EX	300-500	3.16(11)	0	2023±141	2	1.45

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)CH_2CH_3 \rightarrow \text{products}$ Oxygen molecule + 2-Pentene, 2,3-dimethyl-						
73 HUI/HER	RL	298	6.9(-1)			2/2
$k_{ref}: O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow \text{products.}$						
73 HUI/HER	RN	298	5.2(8)			2
$O_2 + CH_3(CH_2)_5CH_3 \rightarrow HO_2 + CH_3(CH_2)_5CH_2$ (a) $\rightarrow HO_2 + CH_3(CH_2)_4CHCH_3$ (b) $\rightarrow HO_2 + CH_3(CH_2)_3CHCH_2CH_3$ (c) $\rightarrow HO_2 + CH_3(CH_2)_2CH(CH_2)_2CH_3$ (d) Oxygen molecule + Heptane						
75 SHA/DEN	EX	397-434	3.16(17)	0	21792±2013	2
$k_a + k_b + k_c + k_d.$						
$O_2(a^1\Delta_g) + CH_2=CHCOOCH_2CH_2CH_2CH_3 \rightarrow \text{products}$ Oxygen molecule + 2-Propenoic acid butyl ester						
79 DAT/RAO	EX	298	(1.36±0.08)(7)			2
Microwave discharge-flow system.						
$O_2(a^1\Delta_g) + CH_3(CH_2)_5CHO \rightarrow \text{products}$ Oxygen molecule + Heptanal						
79 DAT/RAO	EX	298	(6.9±0.1)(6)			2
Microwave discharge-flow system.						
$O_2(a^1\Delta_g) + CH_3COOCH_2CH_2CH(CH_3)_2 \rightarrow \text{products}$ Oxygen molecule + 1-Butanol, 3-methyl-, acetate						
79 DAT/RAO	EX	298	(5.2±1.1)(6)			2
Microwave discharge-flow system.						
$O_2 + $  $\rightarrow $ 						
Oxygen molecule + 1,3-Cyclohexadiene, 5,6-bis(methylene)- $\rightarrow$ 2,3-Benzodioxin, 1,4-dihydro-						
82 ROT/SCH1	EX	461-521	(1.9±1.2)(10)	0	5687±301	2
Thermal reaction in an air thermostat.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
5,6-bis(Methylene)-1,3-cyclohexadiene is in equilibrium with its intermediate form, the bi-radical						
						
(1,2-Phenylenebismethyl) before reacting with O ₂ .						
$O_2(^1\Delta_g) +$  $\rightarrow$ products						
Oxygen molecule + Cyclohexene, 1,2-dimethyl-						
73 HUI/HER	RL	298	4.0(-1)			2/2
$k_{ref}:$						
$O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow$ products.						
73 HUI/HER	RN	298	3.0(8)			2
$O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)CH_2CH_2CH_3 \rightarrow$ products						
Oxygen molecule + 2-Hexene, 2,3-dimethyl						
73 HUI/HER	RL	298	6.6(-1)			2/2
$k_{ref}:$						
$O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow$ products.						
73 HUI/HER	RN	298	5.0(8)			2
$O_2 + (CH_3)_3CCH_2CH(CH_3)_2 \rightarrow HO_2 + (CH_3)_3CCH_2C(CH_3)_2$ (a)						
$\rightarrow HO_2 + (CH_3)_3CCHCH(CH_3)_2$ (b)						
Oxygen molecule + Pentane, 2,2,4-trimethyl-						
73 DEG/DEN	EX	400-465	1.0(15)	0	19124	2
$k_a + k_b.$						
$O_2(^1\Delta_g) + CH_3CH_2OCH=C(CH_2CH_3)CH_2CH_2CH_2CH_3 \rightarrow$ products						
Oxygen molecule + 1-Hexene, 1-ethoxy-2-ethyl-						
73 HUI/HER	RL	298	~5.0(-1)			2/2
Estimated ratio.						
$k_{ref}:$						
$O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow$ products.						
73 HUI/HER	RN	298	~4.0(8)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O₃ (+ M) → O₂ + O (+ M)						
Ozone						
79 END/GLA M = N ₂ . M-efficiencies relative to N ₂ are: 1.29(He), 0.79(Ne), 0.46(Ar), 0.66(Kr), 0.51(Xe), 1.00(N ₂), 0.94(O ₂), 3.86(CO ₂), 2.43(CF ₄), 6.43(SF ₆). Thermal dissociation in shock-waves. Rate constants expressed as k[M].	EX	800	3.5(8)			2
79 HEI/COF M = O ₃ . Critical evaluation.	EX	300-3000	4.32(14)	0	11173	2
80 KLA/LAU M = O ₂ (a ¹ Δ _g , v>1). Flash-photolysis of Ozone. Absorption-Spectroscopy. Resonance-fluorescence. Upper-limit k.	EX	298	≤3.01(11)			2
80 TOB/ULL M = CO ₂ . Vacuum system. P < 1.0×10 ⁻⁵ torr.	EX	348-433	2.00(15)	0	11726±705	2 7.94
82 EGO/POP M = O ₃ . Thermolysis of O ₃ in a static system. P = (75-100) torr.	EX	423	1.87(3)			2
O₃ + SO → O₂ + SO₂						
Ozone + Sulfur monoxide						
80 ROB/SMI Pulsed laser photolysis of O ₃ in excess N ₂ and in presence of COS. P(Total) = 100 torr.	EX	296	(5.24±0.96)(10)			2
82 BLA/SHA1 ¹)	EX	298	(6.38±0.96)(10)			2
82 BLA/SHA2 ¹)	EX	230-420	2.89(13)	0	1170±120	2 1.33
¹) SO generated by ArF laser-photodissociation of SO ₂ at 193 nm. in He diluent. P(SO ₂) ~ 30 mtorr. P(O ₂) < 550 torr. P(O ₃) < 0.4 torr. P(He) = 200 torr.						
O₃(v=n) + SO → O₂ + SO₂(¹B₁)						
Ozone + Sulfur monoxide						
74 KAL/BRA O ₃ [†] produced by CO ₂ laser radiation. k _{ref} : O ₃ + SO → O ₂ + SO ₂ (¹ B ₁).	RL	300	(2.4±0.6)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$O_3 + SO_2 \rightarrow O_2 + SO_3$							
Ozone + Sulfur dioxide							
74 DAV/PRU Upper-limit k.	EX	300	$\leq 6.02(1)$			2	
$O_3 + H_2S \rightarrow HO_2 + HSO$ (a) $\rightarrow OH + HSO_2$ (b)							
Ozone + Hydrogen sulfide							
75 BEC/INO $k_a + k_b$. Upper-limit k. Unreported T assumed to be 298 K.	EX	298	$< 1.20(4)$			2	
75 GLA/TOB1 $k_a = k_b$.	ES	298	5.0(5)			2	
75 GLA/TOB1 $k_a + k_b$.	ES	293-343	1.26(11)	0	3422 $\pm$ 302	2	2.51
75 GLA/TOB2 $k_a + k_b$.	EX	298-343	1.58(14)	0	2617 $\pm$ 604	2	6.31
$O_3 + NO \rightarrow O_2 + NO_2(^2A_1)$ (a) $\rightarrow O_2 + NO_2(^2A_1)$ (b) $\rightarrow O_2 + NO_2(^2B_{1,2})$ (c)							
$O_3 + NO^{\dagger} \rightarrow O_2 + NO_2(^2A_1)$ (d) $\rightarrow O_2 + NO_2(^2B_{1,2})$ (e)							
$O_3^{\dagger} + NO \rightarrow O_2 + NO_2(^2A_1)$ (f) $\rightarrow O_2 + NO_2(^2A_1)$ (g) $\rightarrow O_2 + NO_2(^2B_{1,2})$ (h) $\rightarrow O_3 + NO$ (i)							
Ozone + Nitrogen oxide (NO)							
73 GH0/ELL k_a .	EX	298	(8.5 $\pm$ 0.1)(9)			2	
73 STE/NIK1 k_a .	EX	298	(1.04 $\pm$ 0.06)(10)			2	
74 BEC/SCH k_a .	EX	290	1.02(10)			2	
74 BEM/CLY k_a .	EX	298	(1.09 $\pm$ 0.08)(10)			2	
75 HUI/HER2 k_a . Tubular flow reactor. Mass-spectrometer.	EX	224-364	(2.09 $\pm$ 0.24)(12)	0	1533 $\pm$ 32	2	
75 WU/NIK k_a . NO_2 Photolysis.	EX	298	1.11(10)			2	
76 BIR/SHO k_a .	EX	203-361	(1.41 $\pm$ 0.14)(12)	0	1450 $\pm$ 50	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 FRE/STE $k_a + k_c + k_f + k_h$. $O_3^\dagger = O_3(001)$ (asymmetric stretch.)	EX	298	(1.46±0.15)(11)			2
76 STE/FRE $(k_a + k_c + k_f)/k_a$. Upper-limit ratio.	RL	298	≤2.2(1)			2/2
80 LIP/JES k_a . Stainless-steel reactor. P < 0.1 mtorr.	EX	283-443	(2.59±0.36)(12)	0	1598±50	2
81 MIC/ALL k_a . Fast-flow. Induced fluorescence detection of [NO].	EX	195-369	(1.57±0.48)(12)	0	1435±64	2
81 RAY/WAT ¹)	EX	212-422	(1.90±0.54)(12)	0	1556±80	2
81 RAY/WAT ¹)	EX	299	(1.08±0.05)(10)			2
¹) k_a . Discharge-flow Mass-Spectrometry. $[O_3]_0 = (0.05-1.82) \times 10^{12}$ molec.cm ⁻³ $[NO]_0 = (0.07-1.94) \times 10^{16}$ molec.cm ⁻³						
81 SCH/LIP k_a . Spherical reactor. (7-120)×10 ⁻⁶ torr.	EX	283-433	(1.37±0.24)(12)	0	1475±62	2
82 BOR/BIR ²) Preexponential factor expressed as: $A(T/298)^{2.2}$.	EX	200-350	(1.49±0.15)(11)	2.2	765±116	2
82 BOR/BIR ²) ²) k_a . Reaction of NO with O ₃ in He, by using a dual flow-tube technique. Mass-spectrometry. $[O_3] = (0.05-1.00) \times 10^{13}$ molec.cm ⁻³ . $[NO] = (0.5-6.0) \times 10^{15}$ molec.cm ⁻³ .	EX	298	(1.14±0.11)(10)			2
81 SCH/LIP k_c . Spherical reactor. (7-120)×10 ⁻⁶ torr.	EX	283-433	(1.75±0.18)(12)	0	1951±34	2
78 BAR/MOY ³)	EX	158	(1.06±0.08)(11)			2
78 BAR/MOY ³)	EX	225	(7.5±1.1)(10)			2
78 BAR/MOY ³)	EX	296	(9.2±0.4)(10)			2
78 BAR/MOY ³)	EX	300	9.9(10)			2
78 BAR/MOY ³)	EX	345	(1.24±0.07)(11)			2
78 BAR/MOY ³)	EX	437	(1.85±0.16)(11)			2
³) $k_d + k_e + k_i$. $O_3^\dagger$ is either O ₃ (001) (asymmetric stretch), or O ₃ (010) (bending mode), but not both. Other rate constants within the (158-437) K range are given. Non-Arrhenius behaviour. The k is minimum at 225K. Laser-enhanced fluorescence.						
76 STE/FRE k_e/k_c . NO [†] is NO(v=1).	RL	298	5.7			2/2 1.45
76 GOR/LIN k_f . $O_3^\dagger = O_3(001)$ (asymmetric stretch.) Fit of experimental data to a proposed mechanism.	ES	308	(5.4±0.7)(10)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 KUR/BRA k_f . $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	ES	153-373	2.23(13)	0	1610	2
75 KUR/BRA k_f . $O_3^\dagger = O_3(001) + O_3(100)$ (asymmetric + symmetric stretch.) Fit of experimental data to a proposed mechanism.	ES	153-373	1.20(13)	0	1107	2
75 KUR/BRA k_f . $O_3^\dagger = O_3(001) + O_3(010) + O_3(100)$. (Sum of all three vibrational modes: asymmetric stretch + bend + symmetric stretch.) Fit of experimental data to a proposed mechanism.	ES	153-373	1.20(13)	0	1525	2
77 MOY/BAR k_f/k_a . $O_3^\dagger = O_3(001)$ (asymmetric stretch.) Pulsed CO_2 laser.	RL	153-303	(8.7±2.1)(-1)	0	-649±55	2/2
73 GOR/LIN k_g . $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	ES	350	(1.5±0.2)(11)			2
73 GOR/LIN k_g/k_b . $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	RL	350	≈2.2(1)			2/2
74 KUR/BRA k_g/k_c . $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	RL	300	(1.71±0.43)(1)			2/2
74 KUR/BRA ($k_g + k_h$)/($k_b + k_c$). $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	RL	300	(1.62±0.40)(1)			2/2
74 KUR/BRA $k_g + k_b$. $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	EX	300	(1.63±0.06)(11)			2
78 HUI/COO2 k_g . $O_3^\dagger = O_3(001) + O_3(010) + O_3(100)$. Sum of all three vibrational modes, of which (001) and (100), - asymmetric and symmetric stretch-, are predominant.) Laser-enhanced fluorescence method.	EX	138-410	(2.29±0.54)(11)	0	518±131	2
76 GOR/LIN k_h . $O_3^\dagger = O_3(001)$ (asymmetric stretch.) Fit of experimental data to a proposed mechanism.	ES	308	(4.3±0.7)(9)			2
74 KUR/BRA k_h/k_c . $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	RL	300	(4.1±2.0)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
74 BRA/KUR k_h/k_c . $O_3^{\dagger} = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism. The authors suggest that the $NO_2^*(^2B_2)$ electronic state might very well be the primary emission source, instead of the $^2B_1$ state.	RL	300	(5.6±1.0)			2/2
77 MOY/BAR k_h/k_c . $O_3^{\dagger} = O_3(001)$ (asymmetric stretch.)	RL	153-303	(7.6±2.1)			2/2
77 MOY/BAR k_h/k_c . $O_3^{\dagger} = O_3(001)$ (asymmetric stretch.)	RL	153-303	(8.7±5.5)(-1)	0	-649±126	2/2
78 HUI/COO2 k_h . $O_3^{\dagger} = O_3(001) + O_3(010) + O_3(100)$. (Sum of all three vibrational modes, of which (001) and (100), - asymmetric and symmetric stretch-, are predominant.) Laser-enhanced fluorescence method.	EX	138-410	(6.02±0.18)(11)	0	1449±211	2
75 KUR/BRA k_i . $O_3^{\dagger} = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	ES	153-373	6.02(10)	0	39.2	2
$O_3 + NO_2 \rightarrow O_2 + NO_3$ Ozone + Nitrogen oxide (NO_2)						
73 STE/NIK1	EX	298	(3.91±0.48)(7)			2
73 WU/MOR	EX	299	2.65(7)			2 1.15
74 BEC/SCH	EX	289	1.95(7)			2
74 DAV/PRU	EX	260-343	(5.42±0.49)(10)	0	2428±116	2
74 GHO/ELL Corrected rate constant from 73 GHO/ELL.	EX	298	(1.9±0.3)(7)			2
74 GRA/JOH	EX	231-298	(8.07±0.66)(10)	0	2466±30	2
74 HUI/HER	EX	259-362	(9.44±2.46)(10)	0	2509±76	2
75 GRA	EX	231-298	(8.07±0.66)(10)	0	2466±30	2
75 HER/HUI	EX	259-363	(9.44±2.46)(10)	0	2509±76	2
$O_3 + HONO \rightarrow O_2 + HONO_2$ Ozone + Nitrous acid						
77 KAI/JAP ¹⁾	EX	226	≤3.01(5)			2
77 KAI/JAP ¹⁾	EX	300	≤6.02(4)			2
¹⁾ Upper limit k's. Pyrex reactor in evacuated chamber. P(Total) = (20-30) torr.						
79 STR/WEL Tunable diode-laser. Static reactor. Upper-limit k.	EX	296	≤(2.71±1.81)(5)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
O₃ + CH₄ → products						
Ozone + Methane						
73 STE/NIK2 Upper-limit k.	EX	298	≤7.22(2)			2
O₃ + HCHO → OH + HCO₃ (a) → HO₂ + HCO₂ (b)						
Ozone + Formaldehyde						
76 BRA/HEI k _a + k _b . Upper-limit k.	EX	298	→1.26			2
O₃ + CH₃ONO → O₂ + CH₃ONO₂						
Ozone + Nitrous acid methyl ester (Methyl nitrite)						
76 HAS/FRE	EX	298-352	4.07(11)	0	5315±172	2 1.70
O₃ + CH≡CH → products						
Ozone + Ethyne						
71 DEM	EX	294	(1.8±0.3)(4)			2
73 STE/NIK2	EX	298	(5.18±0.54)(4)			2
76 PAT/ATK1	EX	297	(2.29±0.36)(4)			2
O₃ + CH₂=CH₂ → [C₂H₄.O₃][†] → CH₂OO[†] + HCHO (a) → any other products (b)						
Ozone + Ethene						
80 SU/CAL ¹⁾	EX	298	(1.08±0.06)(6)			2
81 KAN/SU ¹⁾	EX	282-303	1.55(10)	0	2828±181	2 1.86
¹⁾ k _a . Fourier-transform IR-spectroscopy in O ₂ /N ₂ mixtures. P(Total) = 700 torr. The biradical decomposes further to other products.						
73 STE/WU k _{overall} .	EX	299	(9.34±0.90)(5)			2
74 BEC/SCH ²⁾	EX	280-360	7.23(9)	0	2491±101	2
74 BEC/SCH ²⁾	EX	298	1.69(6)			2
²⁾ k _{overall} .						
74 FIN/PIT k _{overall} . In O ₂ carrier gas.	EX	298	(1.0±1.0)(6)			2
74 FIN/PIT k _{overall} . In N ₂ carrier gas.	EX	298	(5.0±2.0)(6)			2
74 HER/HUI k _{overall} .	EX	235-362	(5.42±3.19)(9)	0	2557±167	2
74 JAP/WU2 k _{overall} .	EX	298	(1.14±0.06)(6)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 JAP/WU k _{overall} . In 760 torr. Air.	EX	299	(1.14±0.06)(6)			2
76 JAP/WU k _{overall} . In 760 torr. He.	EX	299	(1.56±0.12)(6)			2
76 TOB/TOB k _{overall} .	EX	303	(1.02±0.08)(6)			2
76 WIL k _{overall} .	EX	298	8.8(5)			2
81 ADE/KER ³⁾	EX	260	2.65(5)			2
81 ADE/KER ³⁾	EX	294	9.64(5)			2
81 ADE/KER ³⁾ Tentative k.	EX	260-294	~1.9(10)	0	~2919	2
³⁾ k _{overall} . Reaction carried out in two Tedlar plastic bags, in synthetic air. Gas-chromatography. P ~ 760 torr.						
82 ATK/ASC1 k _{overall} . Reaction of O ₃ with Ethene in a Teflon bag. Gas-chromatography. [O ₃] < 2.4x10 ¹³ molec.cm ⁻³ .	EX	296	(8.61±1.14)(5)			2
O ₃ + cis-CDH=CDH → [C ₂ D ₂ H ₂ .O ₃] [†] → CDHOO [†] + HCDO Ozone + Ethene-1,2-d ₂ , (Z)-						
80 SU/CAL FTIR Spectroscopy in O ₂ /N ₂ mixtures. The biradical decomposes further to other products. P(Total) = 700 torr.	EX	298	(1.33±0.24)(6)			2
O ₃ + trans-CDH=CDH → [C ₂ D ₂ H ₂ .O ₃] [†] → CDHOO [†] + HCDO Ozone + Ethene-1,2-d ₂ , (E)-						
80 SU/CAL FTIR Spectroscopy in O ₂ /N ₂ mixtures. The biradical decomposes further to other products. P(Total) = 700 torr.	EX	298	(1.33±0.06)(6)			2
O ₃ + CD ₂ =CD ₂ → [C ₂ D ₄ .O ₃] [†] → CD ₂ OO [†] + DCDO Ozone + Ethene-d ₄						
74 JAP/WU2	EX	298	(1.38±0.06)(6)			2
80 SU/CAL FTIR spectroscopy in O ₂ /N ₂ mixtures. The biradical decomposes further to other products. P(Total) = 700 torr.	EX	298	(1.26±0.06)(6)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O₃ + CH₃CHO → products						
Ozone + Acetaldehyde						
73 STE/NIK2	EX	298	(2.05±0.30)(4)			2
81 ATK/ASC	EX	296	≤3.61(3)			2
Reaction in a Teflon bag, in ultra-high purity air. Upper-limit k. P(Total) = 735 torr.						
O₃ + $\triangle$ → CH₂=CH₂ + SO₂						
+ HCHO + CO ₂ (major products)						
Ozone + Thiirane (Ethylene episulfide)						
80 MAR/HER	EX	296	<1.0(4)			2
Stopped-flow autocatalytic reaction. Mass-spectrometry. Upper-limit k. P(Total) = 8 torr.						
O₃ + CH₃CH₂ONO → O₂ + CH₃CH₂ONO₂						
Ozone + Nitrous acid methyl ester						
76 HAS/FRE	EX	298-352	1.90(8)	0	2351±116	2 1.45
O₃ + CH₃C≡CH → products						
Ozone + 1-Propyne						
71 DEM	EX	294	(1.3±0.7)(4)			2
O₃ + CH₂=C=CH₂ → [CH₂=C=CH₂.O₃] → products						
Ozone + 1,2-Propadiene						
74 TOB/TOB	ES	499-598	1.0(9)	0	2768±503	2 5.01
O₃ + CH₃CH=CH₂ → products						
Ozone + 1-Propene						
72 COX/PEN	EX	295	7.6(6)			2
73 STE/WU	EX	299	(7.53±0.60)(6)			2
74 BEC/SCH	EX	280-360	6.63(9)	0	1968±101	2
74 BEC/SCH	EX	298	8.73(6)			2
74 HER/HUI	EX	235-362	(3.70±1.42)(9)	0	1897±109	2
74 JAP/WU2	EX	299	(7.82±0.60)(6)			2
76 JAP/WU	EX	299	(7.95±0.18)(6)			2
In 760 torr. Air.						
76 JAP/WU	EX	299	(1.01±0.06)(7)			2
In 760 torr. He.						
76 WIL	EX	298	5.79(6)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 ADE/KER ¹⁾	EX	260	3.07(6)			2
81 ADE/KER ¹⁾	EX	294	7.59(6)			2
81 ADE/KER ¹⁾ Tentative k.	EX	260-294	~7.58(9)	0	~2013	2
¹⁾ Reaction in two Tedlar plastic bags, in synthetic air. Gas-chromatography. P ~ 760 torr.						
82 ATK/ASC1 Reaction of O ₃ with 1-Propene in a Teflon bag. Gas-chromatography. [O ₃] < 2.4x10 ¹³ molec.cm ⁻³ .	EX	296	(6.26±0.84)(6)			2
O ₃ + CD ₃ CD=CD ₂ → products						
Ozone + Propene-d ₆						
74 JAP/WU2	EX	298	(9.09±0.18)(6)			2
O ₃ + CH ₂ =CHCHO → products						
Ozone + 2-Propenal (Acrolein)						
81 ATK/ASC Reaction in a Teflon bag, in ultrahigh-purity air. P(Total) = 735 torr.	EX	296	(1.69±0.30)(5)			2
O ₃ + CH ₃ C(O)CHO → products						
Ozone + Propanal, 2-oxo-						
76 PAT/ATK1	EX	297	(6.63±3.01)(2)			2
81 ATK/ASC Reaction in a Teflon bag, in ultrahigh-purity air. Upper-limit k. P(Total) = 735 torr.	EX	296	<4.22(4)			2
O ₃ + CH ₂ =CHCN → products						
Ozone + 2-Propenenitrile (Acrylonitrile)						
82 ATK/ASC1 Reaction of O ₃ with 2-Propenenitrile in a Teflon bag. Gas-chromatography. Upper-limit k. [O ₃] < 2.4x10 ¹³ molec.cm ⁻³ .	EX	296	<6.02(4)			2
O ₃ + CH ₃ CH ₂ C≡CH → products						
Ozone + 1-Butyne						
71 DEM	EX	294	(2.4±0.8)(4)			2
O ₃ + CH ₃ C≡CCH ₃ → products						
Ozone + 2-Butyne						
71 DEM	EX	294	(2.0±0.3)(4)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O₃ + CH₂=CHCH=CH₂ → products						
Ozone + 1,3-Butadiene						
74 BEC/SCH	EX	280-360	3.28(10)	0	2682±101	2
74 BEC/SCH	EX	298	4.04(6)			2
74 JAP/WU2	EX	298	(5.06±0.12)(6)			2
75 TOB/TOB	EX	273-343	6.31(10)	0	2919±403	2 3.16
O₃ + CH₃CH₂CH=CH₂ → products						
Ozone + 1-Butene						
74 JAP/WU2	EX	298	(7.41±0.24)(6)			2
75 HUI/HER1	EX	225-363	1.77(9)	0	1686±20	2 1.08
In 0.0015 torr. of O ₂ as scavenger.						
76 WIL	EX	298	5.6(6)			2
81 ADE/KER ¹⁾	EX	260	3.19(6)			2
81 ADE/KER ¹⁾	EX	294	7.59(6)			2
81 ADE/KER ¹⁾	ES	260-294	~6.02(9)	0	~1963	2
¹⁾ Reaction in two Tedlar plastic bags, in synthetic air. Gas-chromatography. P ~ 760 torr.						
O₃ + CH₃CH=CHCH₃ → products						
Ozone + 2-Butene						
74 BEC/SCH	EX	280-360	5.66(9)	0	1147±75	2
74 BEC/SCH	EX	298	1.20(8)			2
cis-, and trans-2-Butene mixture.						
O₃ + cis-CH₃CH=CHCH₃ → products						
Ozone + 2-Butene, (Z)-						
72 COX/PEN	EX	295	8.5(7)			2
72 COX/PEN ¹⁾	EX	295	9.0(7)			2
74 FIN/PIT ¹⁾	EX	298	(1.5±0.2)(8)			2
¹⁾ In N ₂ carrier gas.						
74 FIN/PIT	EX	298	(6.3±1.9)(7)			2 1.3
In O ₂ carrier gas.						
74 JAP/WU2	EX	298	(9.70±0.42)(7)			2
75 HUI/HER1	EX	225-336	1.87(9)	0	956±54	2 1.22
In 0.0075 torr. of O ₂ as scavenger.						
76 WIL	EX	298	7.3(6)			2
O₃ + trans-CH₃CH=CHCH₃ → products						
Ozone + 2-Butene, (E)-						
72 COX/PEN	EX	295	1.55(8)			2
73 STE/WU	EX	299	(1.66±0.14)(8)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
74 JAP/WU2	EX	298	(1.57±0.05)(8)			2	
75 HUI/HER1 In 0.0075 torr. of O ₂ as scavenger.	EX	225-363	3.59(9)	0	1051±43	2	1.17
76 JAP/WU In 760 torr. Air.	EX	299	(1.54±0.09)(8)			2	
76 JAP/WU In 760 torr. He.	EX	299	(1.70±0.04)(8)			2	
81 ADE/KER Reaction in two Tedlar plastic bags, in synthetic air. Gas-chromatography. P ~ 760 torr.	EX	294	1.73(8)			2	
O₃ + (CH₃)₂C=CH₂ → products							
Ozone + 1-Propene-, 2-methyl-							
74 BEC/SCH	EX	283	1.08(7)			2	
74 FIN/PIT In O ₂ carrier gas.	EX	298	(5.4±2.3)(6)			2	
74 FIN/PIT In N ₂ carrier gas.	EX	298	(3.6±0.6)(7)			2	
75 HUI/HER1 In 0.0075 torr. of O ₂ as scavenger.	EX	225-363	1.91(9)	0	1671±23	2	1.06
74 JAP/WU2	EX	298	(8.19±0.12)(6)			2	
76 WIL	EX	298	7.4(6)			2	
81 ADE/KER Reaction in two Tedlar plastic bags, in synthetic air. Gas-chromatography. P ~ 760 torr.	EX	294	7.23(6)			2	
O₃ + CH₃CH=CHCHO → products							
Ozone + 2-Butenal (Crotonaldehyde)							
81 ATK/ASC Reaction in a Teflon bag, in ultrahigh- purity air. P(Total) = 735 torr.	EX	296	(5.42±1.08)(5)			2	
O₃ + CH₃C(O)CH=CH₂ → products							
Ozone + 3-Buten-2-one							
81 ATK/ASC Reaction in a Teflon bag, in ultrahigh- purity air. P(Total) = 735 torr.	EX	296	(2.87±0.36)(6)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$O_3 + CH_2=C(CH_3)CHO \rightarrow$ products							
Ozone + 2-Propenal, 2-methyl- (Methacrolein)							
81 ATK/ASC Reaction in a Teflon bag, in ultrahigh-purity air. P(Total) = 735 torr.	EX	296	(6.75±0.78)(5)			2	
$O_3 +$  (+ M) → adduct							
Ozone + Thiophene							
77 KAD/TOB ¹⁾	EX	303-356	6.31(10)	0	4227±352	2	3.16
77 KAD/TOB ¹⁾ M = O ₂ .	EX	303-356	2.51(18)	0	2365±201	3	2.51
¹⁾ High vacuum reaction vessel. P(Thiophene) ≤1.0 torr. P(O ₃) ≤0.3 torr.							
$O_3 + CH_2=C(CH_3)CH=CH_2 \rightarrow$ products							
Ozone + 1,3-Butadiene, 2-methyl- (Isoprene)							
81 ADE/KER ¹⁾	EX	260	9.94(6)			2	
81 ADE/KER ¹⁾	EX	294	4.22(6)			2	
¹⁾ Reaction in two Tedlar plastic bags, in synthetic air. Gas-chromatography. P ~760 torr.							
82 ATK/WIN Reaction in a thermostated environmental chamber. [O ₃] = (4.7-9.5)×10 ¹² molec.cm ⁻³ .	EX	276-324	9.28(9)	0	2153±430	2	
$O_3 +$  → products							
Ozone + Cyclopentene							
74 JAP/WU2	EX	298	(4.89±0.48)(8)			2	
81 ADE/KER ¹⁾	EX	260	3.45(8)			2	
81 ADE/KER ¹⁾	EX	294	5.84(8)			2	
¹⁾ Reaction in two Tedlar plastic bags, in synthetic air. P ~760 torr. Gas-chromatography.							
$O_3 + CH_3CH_2CH_2CH=CH_2 \rightarrow$ products							
Ozone + 1-Pentene							
74 JAP/WU2	EX	298	(6.44±0.24)(6)			2	
$O_3 +$ cis-CH₃CH₂CH=CHCH₃ → products							
Ozone + 2-Pentene, (Z)-							
72 COX/PEN	EX	295	1.26(8)			2	

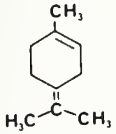
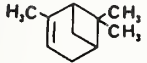
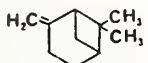
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$O_3 + \text{trans-CH}_3\text{CH}_2\text{CH=CHCH}_3 \rightarrow \text{products}$							
Ozone + 2-Pentene, (E)-							
72 COX/PEN	EX	295	1.9(7)				2
$O_3 + \text{CH}_3\text{CH=C(CH}_3)_2 \rightarrow \text{products}$							
Ozone + 2-Butene, 2-methyl-							
72 COX/PEN	EX	295	4.8(8)				2
74 JAP/WU2	EX	298	(2.97±0.10)(8)				2
75 HUI/HER1	EX	227-363	3.82(9)	0	826±78		1.32
In 0.0075 torr. of O_2 as scavenger.							
$O_3 + \text{CH}_3\text{C(O)CH=CHCH}_3 \rightarrow \text{products}$							
Ozone + 3-Penten-2-one							
81 ATK/ASC	EX	296	(1.28±0.23)(7)				2
Reaction in a Teflon bag, in ultrahigh-purity air. P(Total) = 735 torr.							
$O_3 + \text{Cyclohexene} \rightarrow \text{products}$							
Ozone + Cyclohexene							
74 JAP/WU1	EX	298	(1.02±0.06)(8)				2
M = Air. Ozonolysis of Cyclohexene in a static reactor. Same data given in 74 JAP/WU2.							
[Cyclohexene] $_0$ = (0.51-1.09)×10 ¹⁴ molec.cm ⁻³ .							
[O ₃] $_0$ = (1.22-6.13)×10 ¹² molec.cm ⁻³ .							
P(Total) = 760 torr.							
81 ADE/KER ¹⁾	EX	260	7.23(8)				2
81 ADE/KER ¹⁾	EX	294	7.11(7)				2
¹⁾ Reaction in two Tedlar plastic bags, in synthetic air. Gas-chromatography.							
P ~ 760 torr.							
$O_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH=CH}_2 \rightarrow \text{products}$							
Ozone + 1-Hexene							
72 COX/PEN	EX	295	8.2(6)				2
72 COX/PEN	EX	295	7.2(6)				2
In N ₂ atmosphere.							
73 STE/WU	EX	299	(6.63±0.90)(6)				2
74 JAP/WU2	EX	298	(6.69±0.18)(6)				2
81 ADE/KER	EX	294	6.50(6)				2
Reaction in two Tedlar plastic bags, in synthetic air. Gas-chromatography.							
P ~ 760 torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 ATK/ASC1 Reaction of O ₃ with 1-Hexene Teflon bag. Gas-chromatography. [O ₃] < 2.4x10 ¹³ molec.cm ⁻³ .	EX	296	(7.29±1.69)(6)			2	
O ₃ + CH ₃ CH ₂ CH ₂ C(CH ₃)=CH ₂ → products Ozone + 1-Pentene, 2-methyl-							
72 COX/PEN	EX	295	1.02(7)			2	
O ₃ + (CH ₃) ₂ CHCH ₂ CH=CH ₂ → products Ozone + 1-Pentene, 4-methyl-							
72 COX/PEN	EX	295	6.4(6)			2	
O ₃ + cis-CH ₃ CH ₂ C(CH ₃)=CHCH ₃ → products Ozone + 2-Pentene, 3-methyl-, (Z)-							
74 JAP/WU2	EX	298	(2.75±0.48)(8)			2	
O ₃ + trans-CH ₃ CH ₂ C(CH ₃)=CHCH ₃ → products Ozone + 2-Pentene, 3-methyl-, (E)-							
74 JAP/WU2	EX	298	(3.39±0.10)(8)			2	
O ₃ + (CH ₃) ₂ C=C(CH ₃) ₂ → products Ozone + 2-Butene, 2,3-dimethyl-							
74 JAP/WU2	EX	298	(9.09±0.48)(8)			2	
75 HUI/HER1 In 0.0075 torr. of O ₂ as scavenger.	EX	227-363	1.70(9)	0	294±196	2	1.73
O ₃ +  → products Ozone + 2-Cyclohexen-1-one							
81 ATK/ASC Reaction in a Teflon bag, in ultrahigh-purity air. P(Total) = 735 torr.	EX	296	(7.35±1.57)(5)			2	
O ₃ + CH ₃ (CH ₂) ₄ CH=CH ₂ → products Ozone + 1-Heptene							
82 ATK/ASC1 Reaction in a Teflon bag. Gas-chromatography. [O ₃] < 2.4x10 ¹³ molec.cm ⁻³	EX	296	(1.04±0.17)(7)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O_3 +$  $\rightarrow$ products						
Ozone + Cyclohexene, 1-methyl-4-(1-methylethylidene)- (Terpinolene)						
74 JAP/WU1 M = Air. Ozonolysis of Terpinolene in a static reactor. P(Total) = 760 torr. [Terpinolene] ₀ = (0.39-2.55)x10 ¹³ molec.cm ⁻³ . [O ₃] ₀ = (0.61-1.47)x10 ¹² molec.cm ⁻³ .	EX	296	(4.40±0.66)(8)			2
$O_3 +$  $\rightarrow$ products						
Ozone + Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl- (α-Pinene)						
74 JAP/WU1 ¹⁾ M = Air. [O ₃] ₀ = (0.61-1.47)x10 ¹² molec.cm ⁻³ . [α-Pinene] ₀ = (0.52-1.32)x10 ¹³ molec.cm ⁻³ .	EX	298	(1.99±0.18)(8)			2
74 JAP/WU1 ¹⁾ M = He. [α-Pinene] ₀ = (1.05-1.14)x10 ¹³ molec.cm ⁻³ . [O ₃] ₀ = (0.61-1.35)x10 ¹² molec.cm ⁻³ . ¹⁾ Ozonolysis of α-Pinene in a static reactor. P(Total) = 760 torr.	EX	298	(2.17±0.18)(8)			2
82 ATK/WIN Reaction in a thermostated environmental chamber. Gas-chromatography. [O ₃] = (4.7-9.5)x10 ¹² molec.cm ⁻³ .	EX	276-324	5.66(8)	0	731±173	2
$O_3 +$  $\rightarrow$ products						
Ozone + Bicyclo[3.1.1]heptane, 6,6-dimethyl- 2-methylene- (β-Pinene)						
82 ATK/WIN Reaction in Teflon bag. Gas-chromatography. [O ₃] = (4.7-9.5)x10 ¹² molec.cm ⁻³ .	EX	296	(1.26±0.30)(7)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{H} + \text{O}_2 (+\text{M}) \rightarrow \text{OH} + \text{O} (+\text{M})$ (a)							
$\rightarrow \text{HO}_2 (+\text{M})$ (b)							
Hydrogen atom + Oxygen molecule							
71 BEL/BRA k_a . Constant tube-area.	ES	1128-1152	2.10(14)	0	8354	2	
71 BEL/BRA k_a . Varying tube-area.	ES	1128-1152	1.44(14)	0	8354	2	
71 BRA/BEL1 k_a .	EX	1150-1400	1.245(14)	0	8203±554	2	1.24
71 BRA/BEL2 k_a . Rankine-Hugoniot measurements in shock-tube at low temperatures.	EX	30-90	1.38(14)	0	8254	2	1.05
71 EBE/HOY k_a .	DE	650-1000	2.3(14)	0	8455	2	
73 KOC/MOI k_a .	EX	913-1473	2.7(14)	0	8354±237	2	1.23
73 SCH1 k_a . Preexponential factor expressed as: $A(T/298)^{-0.907}$.	EX	1250-2500	6.95(14)	-0.907	8369	2	
74 NAM/TRO k_a . E_a not determined. Within the given T-range k increases from 4.82×10^9 to $9.64 \times 10^9 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$.	EX	839-924	4.82(9)			2	
75 BOW1 k_a .	ES	1900-2400	6.0(14)	0	8450	2	
80 CHI/SKI k_a . H_2 oxidation in $\text{H}_2/\text{O}_2/\text{Ar}$ mixtures behind reflected shock-waves. Resonance-absorption Spectroscopy.	EX	925-1825	1.1(14)	0	8107	2	
82 PAM/SKI2 k_a . Reaction of O with H_2 behind reflected shock-waves, in $\text{H}_2/\text{O}_2/\text{Ar}$ mixtures. Resonance-absorption Spectroscopy. $[\text{O}] = 5.42 \times 10^8 - 3.49 \times 10^{12} \text{ molec. cm}^{-3}$. $P = (1.16 - 2.67) \text{ atm}$.	EX	1000-2500	1.2(14)	0	8107	2	
71 GAY/PRA ¹⁾ k_b . Expansion channel experiments.	EX	1950-2575	(9.9±5.0)(14)	0	0	3	
71 GAY/PRA ¹⁾ k_b . Radical overshoot experiments.	EX	1220-2370	(1.2±0.3)(15)	0	0	3	
¹⁾ M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 2.0(N ₂), 18.0(H ₂ O).							
71 HIK/EYR k_b . M = Ar.	EX	298	(5.9±0.7)(15)			3	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
71 OSB k_b . M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 0.27(Ne), 1.27(He), 1.85(Kr), 2.20(H ₂).	EX	298	2.12(15)			3	
72 AHU/MIC k_b . M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 0.2(Ne), 1.2(He), 1.8(Kr), 2.0(H ₂).	EX	298	(2.18±0.15)(15)			3	
72 JAC/HOU k_b . M = Ar.	EX	948-1125	2.3(15)	0	0	3	
72 KUR2 k_b . M = He.	EX	203-404	2.41(15)	0	-238±46	3	1.18
72 KUR2 k_b . M = He. M-efficiencies relative to He are: 1.0(He), 4.56(N ₂).	EX	226	6.93(15)			3	
72 KUR2 k_b . M = He. M-efficiencies relative to He are: 1.0(He), 1.0(Ar), 3.4(N ₂), 15.7(CH ₄).	EX	298	5.70(15)			3	
72 MOO/ALL k_b . M = He. M-efficiencies relative to He are: 1.00(He), 1.04(Ar), 4.26(H ₂).	EX	297	(5.4±0.2)(15)			3	
72 WES/DEH1 k_b .	EX	298	(6.8±1.0)(15)			2	
73 KOC/MOI k_b . M = H ₂ .	EX	913-1473	3.24(15)	0	-770±101	3	1.02
73 PEE/MAH1 k_b . M = O ₂ .	EX	1900	2.5(15)			3	
74 HAC/HOY2 k_b . M = He.	EX	300	(5.0±1.0)(15)			3	
74 WON/DAV k_b . M = Ar.	EX	220-360	(2.45±0.40)(15)	0	-345±64	3	
74 WON/DAV k_b . M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 2.69(N ₂).	EX	220	(1.12±0.07)(16)			3	
74 WON/DAV k_b . M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 0.93(He), 3.0(H ₂), 2.8(N ₂), 22.0(CH ₄).	EX	298	7.73(15)			3	
75 VAS/MAK k_b . M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 1.00(He), 4.08(CO ₂).	RN	300	4.35(15)			3	
76 HAC/WAG k_b . M = He.	EX	293	(9.0±1.0)(15)			3	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
77 SLA k_b . M = N ₂ . M-efficiencies relative to N ₂ are: 1.0(Ar), Ar(0.67).	ES	964-1075	(3.3±0.6)(15)	0	0	3
77 SLA ²⁾ k_b . M = Ar. Best-fit of all available data.	SE	200-2200	7.05(15)	-1.0	0	3
77 SLA ²⁾ k_b . M _{eff} (N ₂) = 3.1 at 300 K, decreasing to 1.5 1.5 above 1000 K. Best fit all available data. ²⁾ Preexponential factor expressed as: A(T/298) ⁿ .	SE	200-2000	2.05(16)	-1.42	0	3
78 CAM/ROG k_b . M = N ₂ . Discharge-flow. P(Total) = (0.2-0.5) kPa.	EX	425	(1.2±0.2)(13)			3
78 HAC/WAG k_b . M = He. Isothermal discharge-flow reactor. P = 3.8 torr.	EX	293	(9.0±1.0)(15)			3
79 ISH/SUG2 k_b . M = H ₂ . Pulse-radiolysis. Absorption-spectroscopy. P = 747 torr. H ₂ + 0.93 torr. O ₂ .	EX	298	(1.09±0.22)(16)			3
79 MOR/HEI k_b/k_{ref} . HCHO photolysis at 313 nm. M = O ₂ + N ₂ + 2CO + 3HCHO. k_{ref} : HCHO + H → CHO + H ₂	RL	298	(6.1±1.8)(5)			3/2
80 CHI/SKI k_b . M = Ar. H ₂ oxidation in H ₂ /O ₂ /Ar mixtures behind reflected shock-waves. Resonance-absorption Spectroscopy.	EX	1000	7.0(14)			3
82 PAM/SKI2 k_b . M = Ar. Reaction of O with H ₂ behind reflected shock-waves in H ₂ /O ₂ /Ar mixtures. Resonance-absorption spectroscopy. [O] = 5.42x10 ⁸ -3.49x10 ¹² molec.cm ⁻³ . P = (1.16-2.67) atm.	EX	1000-2500	4.5(14)	0	505	3
H + O₂(¹Δ_g) → OH + O (principal channel)						
Hydrogen atom + Oxygen molecule						
73 SCH/SCH2	EX	300	(1.51±0.30)(10)			2
82 CUP/TAK Discharge-flow apparatus. EPR-spectrometry. O ₂ (¹ Δ _g) generated by microwave-discharge of O ₂ /Ar mixtures. H atoms generated by microwave-discharge of H ₂ /Ar mixtures.	EX	300-431	(8.79±2.95)(12)	0	2013±101	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
D + O₂ (+ M) → OD + O (+ M) (a)							
→ DO₂ (+ M) (b)							
Deuterium atom + Oxygen molecule							
75 APP/APP k _a . Data fit.	ES	1700-3100	3.13(14)	0	9935	2	1.3
80 CHI/SKI k _a . D ₂ oxidation in D ₂ /O ₂ /Ar mixtures behind reflected shock-waves. Resonance-absorption.	EX	1700-2200	1.6(13)	0	7554	2	
82 PAM/SKI2 k _a . Reaction of O with D ₂ behind reflected shock-waves in D ₂ /O ₂ /Ar mixtures. [O] = 5.42x10 ⁸ -3.49x10 ¹² molec.cm ⁻³ . Resonance-absorption. P = (1.16-2.67) atm.	EX	1000-2500	5.8(13)	0	7554	2	
75 VAS/MAK k _b . M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 1.0(He), 4.0(CO ₂).	EX	300	4.35(15)			3	
79 ISH/SUG2 k _b . M = D ₂ . Pulse-radiolysis. Absorption-Spectroscopy. P = 748 torr. (D ₂ + O ₂)	EX	298	(1.05±0.47)(16)			3	
80 CHI/SKI k _b . M = Ar. D ₂ oxidation in D ₂ /O ₂ /Ar mixtures behind reflected shock-waves. Resonance-absorption.	EX	1000	1.6(14)			3	
82 PAM/SKI2 k _b . M = Ar. Reaction of O with D ₂ behind reflected shock-waves in D ₂ /O ₂ /Ar. Resonance-absorption. [O] = 5.42x10 ⁸ -3.49x10 ¹² molec.cm ⁻³ . P = (1.16-2.67) atm.	EX	1000-2500	2.2(14)	0	505	3	
H + O₃ → OH + O₂ (a)							
→ HO₂ + O (b)							
Hydrogen atom + Ozone							
77 CLY/MON k _a .	EX	298-638	5.95(13)	0	224±26	2	1.26
77 SHA k _a . Preexponential factor expressed as: A(T/298) ^{0.75} .	ES	250-2000	1.64(13)	0.75	0	2	
78 LEE/MIC2 k _a . Flash-photolysis. Resonance-fluorescence.	EX	219-360	(8.01±1.93)(13)	0	449±58	2	
79 KEY k _a . Discharge-flow. Resonance-fluorescence. OH is vibrationally excited, with v ≤ 9.	EX	196-424	(9.03±1.08)(11)	0	499±32	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 FOR/WIE k _a + k _b . M = He. Laser photolysis of O ₃ /H ₂ mixtures. H atoms produced by the reaction: O(¹ D) + H ₂ → OH + H. P(H ₂) = 110 mtorr. P(He) = 20 torr. P(O ₃) = (1.7-3.8) mtorr.	EX	298	(1.69±0.06)(13)			2
H + H (+ M) → H₂ (+ M)						
Hydrogen atom						
71 BEN/BLA M = H ₂ . M-efficiencies relative to H ₂ are: 1.0(H ₂), 1.1(N ₂), 1.3(He), 1.7(Ar), 1.6(CO ₂), 1.7(CH ₄), 9.0(N ₂ O).	EX	298	(3.4±0.5)(15)			3
71 GAY/PRA ¹⁾ Expansion channel experiments.	EX	1950-2575	3.3(14)	0	0	3 1.97
71 GAY/PRA ¹⁾ Radical overshoot experiments.	EX	1220-2370	(3.8±0.5)(14)	0	0	3
¹⁾ M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 1.0(N ₂), 6.0(H ₂ O).						
73 AZA/BOR M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 1.31(He).	EX	298	(4.5±0.7)(15)			3
73 TEN/WIN ²⁾ M = NH ₃ . Based on k _{ref} reported in 71 BEN/BLA.	RN	298	(4.0±0.09)(16)			3
73 TEN/WIN ²⁾ M = NH ₃ . Based on k _{ref} estimated by: Ham, D.Trainer, D.W., and Kaufman, F., in J. Chem. Phys. 53, 4395(1979).	RN	298	5.14(16)			3
²⁾ Determined by adding NH ₃ to He carrier gas, then using the literature values for the H atom recombination in presence of He, to calculate the k in presence of NH ₃ . k _{ref} : H + H + He.						
73 TRA/HAM M = He. M-efficiencies relative to He are: 1.00(He), 1.54(H ₂), 2.28(Ar).	EX	77	(4.35±0.54)(15)			3
73 TRA/HAM M = He. M-efficiencies relative to He are: 1.00(He), 1.16(H ₂), 1.31(Ar).	EX	298	(2.54±0.15)(15)			3
74 MAL/OWE M = Ar.	EX	1300-1700	1.0(15)	0	0	3 1.20

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 WAL/KAU ³⁾ M = H ₂ . n = 0 assumed.	EX	77-298	2.21(15)	0	-86	3	1.1
75 WAL/KAU ³⁾ M = H ₂ .	EX	77-298	2.94(15)	-0.6	0	3	1.1
75 WAL/KAU ³⁾ M = CO ₂ . n = 0 assumed.	EX	175-295	1.01(15)	0	-523	3	1.1
75 WAL/KAU ³⁾ M = CO ₂ .	EX	175-295	5.80(15)	-2.27	0	3	1.1
³⁾ A-factors recalculated from the E _a (or the given n of the T ⁻ⁿ factor) and the experimental k at 298 (or 295) K. The preexponential factors expressed as: A(T/298) ⁿ in all the expressions with n ≠ 0.							
75 WAL/KAU M = H ₂ . M-efficiencies relative to H ₂ are: 1.00(H ₂), 0.65(He), 1.48(Ar), 2.97(N ₂), 3.99(CH ₄).	EX	77	(6.71±0.80)(15)			3	
75 WAL/KAU M = H ₂ . M-efficiencies relative to H ₂ are: 1.00(H ₂), 0.87(He), 1.13(N ₂), 1.14(Ar), 1.89(CH ₄), 2.02(CO ₂), 2.41(SF ₆).	EX	298	(2.94±0.15)(15)			3	
76 LYN/SCH M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.61(Ne), 0.72(He), 0.83(Ar), 0.89(H ₂), 1.06(Kr).	EX	298	(3.48±0.51)(15)			3	
77 MIT/LER M = He. About 25% p-H ₂ formed.	EX	297	(2.10±0.07)(15)			3	
78 HAR/KUM ⁴⁾ M = H ₂ . In the presence of H ₂ O vapor traces.	EX	298	(5.44±1.09)(15)			3	
78 HAR/KUM ⁴⁾ M = H ₂ . In the absence of H ₂ O vapor traces.	EX	298	(7.62±2.54)(14)			3	
⁴⁾ Microwave discharge-flow system.							
D + D (+ M) → D₂ (+ M)							
Deuterium atom							
73 AZA/BOR M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 1.38(He).	EX	298	(2.90±0.54)(15)			3	
73 TRA/HAM ¹⁾	EX	77	5.5(15)			3	1.1
73 TRA/HAM ¹⁾	EX	298	2.2(15)			3	1.1
¹⁾ M = D ₂ .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	E, B-B(ref)	k, A units	k err. factor
H + H₂(v=1) → H₂ + H							
Hydrogen atom + Hydrogen molecule							
78 GOR/IVA1 ¹⁾	EX	300	(3.11±0.12)(12)				2
78 GOR/IVA1 ¹⁾	EX	356	(5.61±0.48)(12)				2
¹⁾ Hydrogen maser storage-bulb. Mass-spectrometry. [H ₂] = (0.5-6.5)×10 ¹³ molec.cm ⁻³ .							
H + HD → H₂ + D							
Hydrogen atom + Deuterium hydride							
72 NIK/MAI	CO	1000	(1.39±0.12)(13)				2
H + HD(v=1) → HD + H (a) → H₂ + D (b)							
Hydrogen atom + Deuterium hydride							
78 GOR/IVA1 ¹⁾	EX	300	(4.40±2.05)(12)				2
78 GOR/IVA1 ¹⁾	EX	356	(3.13±1.08)(12)				2
¹⁾ k _a + k _b . Hydrogen maser storage-bulb. Mass-spectrometry. [H ₂] = (0.5-6.5)×10 ¹³ molec.cm ⁻³ .							
H + D₂ → HD + D							
Hydrogen atom + Deuterium molecule							
72 NIK/MAI	CO	1000	(2.77±0.30)(13)				2
75 APP/APP	EX	1860	4.01(12)				2
75 APP/APP	EX	2680	9.40(12)				2
75 APP/APP	EX	2730	1.00(13)				2
76 PRA/ROG1	EX	274-1220	2.01(11)	3.21	2851±88		2 3.39
The preexponential factor expressed as: A(T/298) ^{3.21} .							
H + D₂(v=1) → HD + D							
Hydrogen atom + Deuterium molecule							
75 GOR/IVA ¹⁾	EX	470	(1.42±0.18)(10)				2
[H ₂] = [D ₂] = (0.1-1.0) ¹⁴ molec.cm ⁻³ .							
78 GOR/IVA1 ¹⁾	EX	300	(5.06±0.60)(11)				2
78 GOR/IVA1 ¹⁾	EX	356	(5.48±0.90)(11)				2
[H ₂] = [D ₂] = (0.5-6.5)×10 ¹³ molec.cm ⁻³ . ¹⁾ Hydrogen maser storage-bulb.. Mass-spectrometry.							
D + H₂ → HD + H							
Deuterium atom + Hydrogen molecule							
72 NIK/MAI	CO	1000	(3.67±0.36)(13)				2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
73 MIT/LER The preexponential factor expressed as: $A(T/298)^2$.	EX	167-346	(1.46±0.09)(12)	2.0	2698±20	2
75 APP/APP	EX	2600	1.54(13)			2
76 PRA/ROG1 The preexponential factor expressed as: $A(T/2.5198)^{2.51}$.	EX	274-1220	7.77(11)	2.51	2491±70	2 2.75
D + H₂(v=n) → DH + H						
Deuterium atom + Hydrogen molecule						
82 GLA/CHA ¹⁾ v = 0.	EX	297	(1.51±0.60)(8)			2
82 GLA/CHA ¹⁾ v = 1.	EX	297	(5.90±1.81)(11)			2
¹⁾ Discharge-flow system. EPR-spectrometry.						
D + HD → D₂ + H						
Deuterium atom + Deuterium hydride						
72 NIK/MAI	CO	1000	(1.87±0.18)(13)			2
H + OH (+ M) → H₂O (+ M)						
Hydrogen atom + Hydroxyl						
72 FRI/SUT M = O ₂ , N ₂ . Rate constant expressed as: $k[M] = 4.4 \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$.	ES	2130	4.4(10)			2
77 ZEL/ERL	EX	230-300	1.56(10)	0	0	2 1.2
71 GAY/PRA Expansion channel experiments.	EX	1950-2575	(2.4±0.8)(15)	0	0	3
71 GAY/PRA Radical overshoot experiments.	EX	1220-2370	(2.7±0.7)(15)	0	0	3
¹⁾ M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 4.0(N ₂), 18.0(H ₂ O).						
77 ZEL/ERL M = He. The preexponential factor expressed as: $A(T/298)^{-2.6}$.	EX	230-300	(5.76±4.02)(16)	-2.6	0	3
77 ZEL/ERL M = He. M-efficiencies relative to He are: 1.0(He), 1.5(Ar), 3.2(N ₂), 6.0(CO ₂).	EX	300	(5.44±1.45)(16)			3
D + OH → OD + H						
Deuterium atom + Hydroxyl						
75 MAR/KAU2 Discharge-flow. UV Resonance-fluorescence.	EX	295	(7.83±1.81)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 HOW/SMI Laser flash-photolysis. Time-resolved Resonance-fluorescence. OH generated by pulse Laser-photolysis of HONO ₂ or H ₂ O. D atom generated by D ₂ microwave discharge. The preexponential factor expressed as: $A(T/298)^{-0.63}$.	EX	300-515	(3.15±0.50)(13)	-0.63	0	2
$H + OH + OH \rightarrow H_2O + OH(^2\Sigma)$ Hydrogen atom + Hydroxyl						
74 DAV/MCG	EX	1740-1860	(8.34±0.33)(15)	0	0	3
$H + OH + CO \rightarrow HCHO + O$ Hydrogen atom + Hydroxyl + Carbon monoxide						
78 SME/PAV Shock-waves. Non-Arrhenius expression. 1) $k = 4.35 \times 10^{20} (1/T) \text{ cm}^6 \text{ mol}^{-2} \text{ s}^{-1}$.	EX	1500-3500	1)			3
$H + HO_2 \rightarrow H_2 + O_2$ (a) → OH + OH (b) → H ₂ O + O (c) Hydrogen atom + Hydroperoxo						
71 BEN/BLA k_a/k_b . Estimated ratio.	RL	298	(7.5±2.5)(-1)			2/2
72 WES/DEH1 $k_a/(k_a + k_b + k_c)$. Estimated ratio.	RL	298	6.2(-1)			2/2
74 BAL/FUL1 k_a/k_b . Reaction vessel in electric furnace. Second limit measurement.	RL	773	1.7(-1)			2/2
74 BAL/FUL1 $k_a + k_b$. Reaction vessel in electric furnace. Second limit measurement.	ES	300-773	3.1(14)	0	868	2
76 HAC/WAG $k_a/(k_a + k_b + k_c)$.	RL	293	2.9(-1)			2/2
76 HAC/WAG k_a .	RN	293	(6.7±1.5)(12)			2
77 SHA k_a . The preexponential factor expressed as: $A(T/298)^{0.75}$.	ES	250-2000	8.25(12)	0.75	0	2
78 HAC/WAG 1) k_a/k_b .	RL	293	4.2(-1)			2/2
78 HAC/WAG 1) $k_a/(k_a + k_b + k_c)$.	RL	293	2.9(-1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
78 HAC/WAG ¹⁾ k _a . ¹⁾ Isothermal discharge-flow reactor. P = 3.8 torr.	RN	293	(1.0±0.5)(13)			2
82 SRI/QIU k _a . Discharge-flow reactor. Laser-induced Fluorescence. UV-Resonance-Fluorescence. HO ₂ generated by reacting F with H ₂ O ₂ . F atoms generated by dissociation of CF ₄ in a microwave-discharge. H and O atoms generated by dissociation of H ₂ and O ₂ in a microwave-discharge. [NO] ~ 2x10 ¹⁴ molec.cm ⁻³ . P(He) ~ 2.5 torr. [H] ₀ = [O] ₀ ~ (4-5)x10 ¹⁰ molec.cm ⁻³ . [CF ₄] = (1-10)x10 ¹³ molec.cm ⁻³ . [H ₂ O ₂] = 8x10 ¹² molec.cm ⁻³ .	EX	296	(4.03±2.04)(12)			2
72 DAY/DIX ²⁾	RL	300-1800	(6.5±1.0)	0	0	2/2
73 DAY/THO ²⁾	RL	300-1050	(6.5±1.0)	0	0	2/2
²⁾ (k _b + k _c)/k _a . Estimated ratio.						
72 WES/DEH1 k _b /(k _a + k _b + k _c). Estimated ratio.	RL	298	2.7(-1)			2/2
76 HAC/WAG k _b /(k _a + k _b + k _c).	RL	293	6.9(-1)			2/2
76 HAC/WAG k _b .	RN	293	(1.6±0.8)(13)			2
77 COL/NAE ³⁾ k _{ref} : H + CH ₃ CHO → H ₂ + CH ₃ CO	RL	1113	2.5(-2)			2/2
77 COL/NAE ³⁾ k _{ref} : HO ₂ + CH ₃ CHO → H ₂ O ₂ + CH ₃ CO	RL	1113	2.9(-2)			2/2
77 COL/NAE ³⁾ k _{ref} : H ₂ O ₂ + M → OH + OH + M	RL	1113	3.1(-2)			2/2
³⁾ k _b /k _{ref} .						
77 SHA k _b . The preexponential factor expressed as: A(T/298) ^{0.75} .	ES	250-2000	8.25(12)	0.75	0	2
78 HAC/WAG ⁴⁾ k _b /(k _a + k _b + k _c).	RL	293	6.9(-1)			2/2
78 HAC/WAG ⁴⁾ k _b . ⁴⁾ Isothermal discharge-flow reactor. P = 3.8 torr.	RN	293	(2.5±1.0)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 SRI/QIU k _b . Discharge-flow reactor. Laser-induced Fluorescence. UV-Resonance-Fluorescence. HO ₂ generated by reacting F with H ₂ O ₂ . F, H and O atoms generated by dissociation of CF ₄ , H ₂ and O ₂ , respectively, in a microwave-discharge. P(He) ~ 2.5 torr. [NO] ~ 2x10 ¹⁴ molec.cm ⁻³ . [H] ₀ = [O] ₀ ~ (4-5)x10 ¹⁰ molec.cm ⁻³ . [CF ₄] = (1-10)x10 ¹³ molec.cm ⁻³ . [H ₂ O ₂] = 8x10 ¹² molec.cm ⁻³ .	EX	296	(3.85±0.60)(13)			2
72 WES/DEH1 k _c /(k _a + k _b + k _c). Estimated ratio.	RL	298	1.1(-1)			2/2
76 HAC/WAG k _c /(k _a + k _b + k _c).	RL	293	2.0(-2)			2/2
76 HAC/WAG k _c .	RN	293	5.0(11)			2
78 HAC/WAG ⁵⁾ k _c /(k _a + k _b + k _c).	RL	293	2.0(-2)			2/2
78 HAC/WAG ⁵⁾ k _c . Upper-limit k.	RN	293	≤7.0(11)			2
⁵⁾ Isothermal discharge-flow. P = 3.8 torr.						
82 SRI/QIU k _c . Discharge-flow. Laser-induced Fluorescence. UV-Resonance-Fluorescence. HO ₂ generated by reacting F with H ₂ O ₂ . F, H and O atoms generated by dissociation of CF ₄ , H ₂ and O ₂ , respectively, in a microwave discharge. P(He) ~ 2.5 torr. [NO] ~ 2x10 ¹⁴ molec.cm ⁻³ . [H] ₀ = [O] ₀ ~ (4-5)x10 ¹⁰ molec.cm ⁻³ . [CF ₄] = (1-10)x10 ¹³ molec.cm ⁻³ . [H ₂ O ₂] = 8x10 ¹² molec.cm ⁻³ .	EX	296	(1.81±0.90)(12)			2
77 HAC/PRE k _a + k _b + k _c . Isothermal flow.	EX	293	(3.6±1.0)(13)			2
78 PRE k _a + k _b + k _c . Laser Magnetic Resonance Spectroscopy.	EX	293	(3.2±1.0)(13)			2
79 HAC/PRE1 k _a + k _b + k _c . Isothermal flow. Laser Magnetic Resonance Spectrometry. P(Total) = (130-800) Pa.	EX	293	(2.8±0.6)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 THR/WIL2 $k_a + k_b + k_c$. Laser magnetic Resonance Spectrometry.	EX	298	(3.01±0.78)(13)			2
82 SRI/QIU $k_a + k_b + k_c$. Discharge-flow. Laser-induced Fluorescence. UV-Resonance-Fluorescence. HO ₂ radicals generated by reacting F with H ₂ O ₂ . F, H and O atoms generated by dissociation of CF ₄ , H ₂ , and O ₂ , respectively, in a microwave-discharge. [H] ₀ = [O] ₀ ~ (4-5)×10 ¹⁰ molec.cm ⁻³ . [CF ₄] = (1-10)×10 ¹³ molec.cm ⁻³ . [H ₂ O ₂] = 8×10 ¹² molec.cm ⁻³ . [NO] ~ 2×10 ¹⁴ molec.cm ⁻³ . P(He) ~ 2.5 torr.	EX	296	(4.46±0.72)(13)			2
H + H ₂ O → H ₂ + OH Hydrogen atom + Water						
79 COH/WES Critical review. $k_1 = Kk_{-1}$. The preexponential factor expressed as: $A(T/298)^{1.2}$. $\Delta \log k = 0.1$ at 300 K, and 0.4 at 2000 K.	RE	250-3000	9.52(12)	1.2	9610	2
H + H ₂ O ₂ → H ₂ + HO ₂ (a) → OH + H ₂ O (b) Hydrogen atom + Hydrogen peroxide						
72 VOL/GOR k_b/k_a .	RL	298	(3.0±1.0)			2/2
73 GOR k_a .	ES	298	(2.41±1.20)(8)			2
74 GOR/VOL k_a .	ES	298	(1.87±0.48)(9)			2
75 KLE/PAY $k_a + k_b$. Channel (b) assumed to be predominant.	EX	283-353	(3.13±1.20)(12)	0	1399±141	2
72 GOR/VOL k_b/k_a . (Corrected rate ratio.)	RL	298	(2.0±1.0)			2/2
73 GOR k_b/k_a .	RL	298	(3.0±1.0)			2/2
73 GOR k_b .	ES	298	(7.23±0.36)(8)			2
74 GOR/VOL k_b/k_a .	RL	298	(1.86±0.14)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
74 GOR/VOL k_b .	ES	298	(3.4±0.84)(9)			2	
75 MEA/HEI k_b/k_a .	RL	298	1.3			2/2	
$D + H_2O_2 \rightarrow HD + HO_2$ (a) $\rightarrow OH + HDO$ (b)							
Deuterium atom + Hydrogen peroxide							
71 ALB/HOY $k_a + k_b$.	EX	294-464	7.0(12)	0	2114±201	2	
$H + SO_2 \rightarrow HSO_2$							
Hydrogen atom + Sulfur dioxide							
78 GOR/IVA2 ¹⁾	EX	305	1.81(11)			2	
78 GOR/IVA2 ¹⁾	EX	375	2.23(11)			2	
¹⁾ Based on collision-induced shifts and HF-transition line broadening in H atoms.							
$H + SH \rightarrow H_2 + S$							
Hydrogen atom + Mercapto							
72 LAN/OLD Upper-limit k.	ES	293	≤6.02(12)			2	
73 BRA/TRU	EX	298	2.5(13)			2	
75 CUP/GLA	EX	295	(1.51±0.48)(13)			2	
79 NIC/AMO Radio-frequency pulse. Kinetic spectroscopy. Computer simulation. High-vacuum. P = (0.1-2) torr.	DE	295	(1.3±0.2)(13)			2	
$H + H_2S \rightarrow H_2 + SH$							
Hydrogen atom + Hydrogen sulfide							
71 KUR/PET1	EX	190-464	(7.77±0.90)(12)	0	860±30	2	
72 ROM/SCH	EX	298	(2.29±0.24)(11)			2	
73 BRA/TRU	EX	298	5.0(11)			2	
77 FRA/ROG Conventional static system.	EX	808-937	2.75(13)	0	330±220	2	1.78
79 NIC/AMO Radio-frequency pulse. Kinetic Spectroscopy. High-vacuum system. Computer simulation. P = (0.1-2) torr.	DE	295	(5.0±0.4)(11)			2	
80 HUS/SLA1 Time-resolved Resonance-Fluorescence.	EX	300	(5.18±0.30)(11)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 ROT/LOE1 Thermolysis of H ₂ S behind reflected shock-waves. Atomic-resonance Absorption-Spectroscopy. P(Total) = (1350-15000) torr. [H ₂ S] = (0.6-4.9)x10 ¹⁵ molec.cm ⁻³ . [Ar] = (5.0-8.0)x10 ¹⁸ molec.cm ⁻³ .	EX	1965-2560	1.08(13)	0	1500	2
D + D ₂ S → D ₂ + SD Deuterium atom + Hydrogen sulfide (D ₂ S)						
80 HUS/SLA1 Time-resolved Resonance-Fluorescence.	EX	300	(4.76±0.24)(11)			2
H + N (+ M) → NH (+ M) Hydrogen atom + Nitrogen atom						
73 BRO Central k value by averaging: k < (6.4±1.5)x10 ⁻³² cm ⁶ molec ⁻² s ⁻¹ and k > (3.1±1.0)x10 ⁻³² cm ⁶ molec ⁻² s ⁻¹ .	EX	298	(1.82±1.05)(16)			3
H + N ₂ → NH + N Hydrogen atom + Nitrogen molecule						
78 ROO/HAN Shock-waves. The preexponential factor expressed as: A(T/298) ^{0.5} .	ES	1700-3000	5.18(13)	0.5	71465	2
H + NO (+ M) → OH + N (+ M) Hydrogen atom + Nitrogen oxide (NO)						
75 BRA/CRA ¹⁾	DE	2530-3020	3.5(14)	0	23937	2
75 DUX/PRA ¹⁾	DE	2200-3250	2.6(14)	0	24560	2
¹⁾ Optimization based on a proposed mechanism.						
75 FLO/HAN Best fit to the experimental data.	EX	2403-4500	1.34(14)	0	24761±403	2 1.15
75 KOS/AND Data-fit to a proposed mechanism.	ES	2000-4000	3.16(13)	0	24157±151	2 2.0
76 AND/ASA Reevaluation of the experimental data reported in 75 KOS/AND by using computer simulation.	DE	2300-3500	5.01(13)	0	24509	2 1.41
77 FLO/HAN Best data-fit to a proposed mechanism.	EX	2415-4200	2.22(14)	0	25415±302	2 1.20

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 MCC/KRU ²⁾	EX	1750-2040	1.74(14)	0	24761	2	1.58
77 MCC/KRU ²⁾	RE	1750-2040	1.71(14)	0	24560	2	
Based on a curve fit of all previous rate constants. Recommended k.							
²⁾ Flow reactor.							
Same data given in 76 MCC/KRU.							
77 OKA/SIN2	EX	298-477	(4.61±0.16)(15)	0	-363±13	2	
M = H ₂ .							
Photomultiplier with lock-in amplifier.							
81 FOR ³⁾	EX	313	5.01(14)			2	
M = N ₂ . P >400 atm.							
81 FOR ³⁾	EX	313	1.50(14)			2	
M = Ar. P <100 atm. Extrapolation by using the Cassel curve method of Troe.							
³⁾ Steady-state quasi-monochromatic Photolysis of NO/HI mixtures. Limiting high-pressure k's.							
71 HIK/EYR	EX	298	(1.4±0.2)(16)			3	
M = H ₂ .							
71 OSB	EX	298	1.40(16)			3	
M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 0.56(Ne), 1.11(He), 1.40(Kr), 1.63(H ₂).							
72 AHU/MIC	EX	298	(1.41±0.04)(16)			3	
M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 0.5(Ne), 1.1(He), 1.4(Kr), 1.6(H ₂).							
73 ATK/CVE ⁴⁾	EX	285-390	8.9(15)	0	-272±75	3	
73 ATK/CVE ⁴⁾	EX	298	(2.150±0.13)(16)			3	
⁴⁾ M = H ₂ .							
75 CAM/HAN2	EX	392	(8.7±0.7)(15)			3	
M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 1.64(N ₂).							
77 OKA/SIN1	EX	298	(1.56±0.06)(16)			3	
M = H ₂ .							
77 OKA/SIN2 ⁵⁾	EX	298	(1.55±0.23)(16)			3	
M = H ₂ .							
77 OKA/SIN2 ⁵⁾	EX	298	(1.91±0.38)(16)			3	
M = NO.							
⁵⁾ Photomultiplier with lock-in amplifier.							
79 ISH/SUG2	EX	298	(1.66±0.22)(16)			3	
M = H ₂ . Pulse-radiolysis.							
Absorption-spectroscopy.							
P = (100-300) torr. H ₂ + (0.05-0.65) torr. NO							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
D + NO (+ M) → DNO (+ M)							
Deuterium atom + Nitrogen oxide (NO)							
79 ISH/SUG2 M = D ₂ . Pulse-radiolysis. Absorption-spectroscopy. P = (100-900) torr. (D ₂ + NO)	EX	298	(1.60±0.36)(16)			3	
H + NO₂ → OH + NO							
Hydrogen atom + Nitrogen oxide (NO ₂)							
76 WAG/WEL	EX	240-460	(4.3±1.8)(14)	0	505±84	2	
77 BEM/CLY	EX	298	(6.81±1.39)(13)			2	
77 CLY/MON	EX	298-653	2.89(14)	0	174±31	2	1.21
79 MIC/NAV2 T-independent. Mean value of two techniques: Flash-photolysis-, and Discharge-flow- Resonance-fluorescence.	EX	195-400	(8.49±1.57)(13)	0	0	2	
81 AGR/MAN Flowing-afterglow apparatus. Rotationless Einstein coefficient of Rosmus. P(Ar) = 0.7 torr.	EX	300	7.53(13)			2	
H + N₂O → OH + N₂ (a) → NH + NO (b)							
Hydrogen atom + Nitrogen oxide (N ₂ O)							
73 BAL/GET k _a /k _{ref} . k _{ref} : H + O ₂ → OH + O.	RL	773	(6.4±0.7)(-1)			2/2	
73 BAL/GET ¹⁾	RN	773	2.6(9)			2	1.4
73 BAL/GET ¹⁾ ¹⁾ k _a .	SE	460-2500	7.6(13)	0	7599±503	2	
73 WAL1 k _a /k _{ref} . k _{ref} : H + O ₂ → OH + O.	RL	773	(6.4±0.07)(-1)			2/2	
73 WAL1 ²⁾	RN	773	2.6(10)			2	1.4
73 WAL1 ²⁾ Present and independent data combined. ²⁾ k _a .	SE	700-2503	7.6(13)	0	7599±503	2	
75 ALB/HOY k _a .	EX	718-1111	(2.2±0.7)(14)	0	8709±349	2	
77 BAL/VAN k _a . Supersonic molecular beam. Mass-spectrometry. P = 40 torr.	EX	1000-1700	(6.0±2.0)(13)	0	6593	2	
78 DEA/STE k _a . M = Ar. Reflected shock waves. Best fit.	EX	1950-2850	1.81(15)	0	13592	2	
79 GLA/QUY k _a . Discharge-flow shock-tube.	EX	1473-2710	(3.82±0.66)(13)	0	8505±377	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
79 QUY k _a . Shock-tube technique. P < 760 torr.	EX	1475-2875	(3.26±0.47)(13)	0	8153±302	2	
80 DEA/JOH1 k _a . HCHO Decomposition behind shock-waves. Best data fit. Total conc. = 5x10 ¹⁸ molec.cm ⁻³ .	EX	1700-2500	3.31(14)	0	5281	2	
80 MUR/BOR1 ³⁾	RN	1550	9.77(11)			2	
80 MUR/BOR1 ³⁾	RN	1923	1.26(12)			2	
³⁾ k _a . Oxidative pyrolysis of CH ₄ behind reflected shock-waves, initiated by the N ₂ O decomposition. Other k values are given for various T's within (1550-1923) K range. E _a not given. Determined relative to the reaction: H + CH ₄ → H ₂ + CH ₃							
78 BOR/ZAM k _b . Static system. Reflected shock-waves.	EX	850-2000	6.31(13)	0	14595±755	2	2.0
H + N ₂ O(v=3) → OH + N ₂							
Hydrogen atom + Nitrogen oxide (N ₂ O)							
77 GER/EGO Upper-limit k.	EX	298	<6.02(10)			2	
H + NH → H ₂ + N							
Hydrogen atom + Imidogen							
81 MOR2 Premixed H ₂ /O ₂ /Ar flames. Laser-fluorescence. P = 760 torr.	EX	1790	~3.01(13)			2	2.0
H + NH ₂ (+ M) → H ₂ + NH (+ M) (a) → NH ₃ (+ M) (b)							
Hydrogen atom + Amidogen							
71 BOY/WIL k _a . Radiolysis of gaseous NH ₃ . P(NH ₃) = 700 torr.	ES	298	(2.9±0.7)(12)			2	
79 DOV/NIP k _a . Pyrolysis behind reflected shock-waves.	RN	2500-3000	6.17(13)	0	2630	2	
81 YUM/ASA k _a . M = Ar. Thermolysis of NH ₃ behind incident shock-waves. Vacuum-UV Absorption-Spectroscopy. [NH ₃] ₀ = (1.2-2.4)x10 ¹⁴ molec.cm ⁻³ . [Ar] = (0.2-1.8)x10 ¹⁸ molec.cm ⁻³ .	EX	2450-3020	3.02(13)	0	4308	2	
71 BOY/WIL k _b . Radiolysis of gaseous NH ₃ . P(NH ₃) = 700 torr.	ES	298	(1.8±0.4)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
79 PAG/ERI k_D . Gaseous NH_3 pulse-radiolysis.	EX	349	1.6(13)			2	
71 GOR/MUL k_D . Unreported T assumed to be 298 K.	EX	298	2.2(18)			3	
H + $\text{NH}_3 \rightarrow \text{H}_2 + \text{NH}_2$							
Hydrogen atom + Ammonia							
74 DOV/NIP	EX	1500-2150	2.75(13)	0	8757±654	2	1.45
81 YUM/ASA M = Ar. Thermolysis of NH_3 behind incident shock-waves. Vacuum-UV Absorption-Spectroscopy. $[\text{NH}_3]_0 = (0.6-1.8) \times 10^{15} \text{ molec.cm}^{-3}$. $[\text{Ar}] = (0.1-1.2) \times 10^{19} \text{ molec.cm}^{-3}$.	EX	1860-2480	1.24(14)	0	10820±5184	2	11.0
H + $\text{NH}_2\text{NH} \rightarrow \text{NH}_2 + \text{NH}_2$							
Hydrogen atom + Hydrazyl							
71 GEH/HOY	EX	300	(1.6±0.8)(12)			2	
H + $\text{NH}_2\text{NH}_2 \rightarrow \text{H}_2 + \text{NH}_2\text{NH}$							
Hydrogen atom + Hydrazine							
71 FRA/JON	EX	300-540	(1.5±0.3)(12)	0	654±101	2	
71 GEH/HOY	EX	213-473	1.3(13)	0	1258	2	
76 STI/PAY	EX	228-400	(5.94±0.70)(12)	0	1198±50	2	
H + $\text{HN}_3 \rightarrow \text{NH}_2 + \text{N}_2$							
Hydrogen atom + Hydrazoic acid							
73 LEB/COM	EX	300-460	1.53(13)	0	2315	2	
H + $\text{HNO} \rightarrow \text{H}_2 + \text{NO}$							
Hydrogen atom + Nitrosyl hydride							
72 SMI	EX	2100	(2.35±1.14)(12)			2	
75 CAM/HAN2 k_{ref} : O + $\text{HNO} \rightarrow \text{OH} + \text{NO}$. Upper-limit ratio.	RL	425	≤8.86(-3)			2/2	
78 WAS/AKI Fast flow. Lower-limit k. Photoionization Mass-spectrometer.	EX	298	>9.64(11)			2	
80 DOD/ZEL High-frequency discharge. Mass-spectrometry.	EX	295	(7.23±3.00)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
H + HONO₂ → products						
Hydrogen atom + Nitric acid						
74 CHA/WAY Upper-limit k.	EX	300	≤1.20(9)			2
H + HO₂NO₂ → products						
Hydrogen atom + Peroxynitric acid						
81 TRE/BAR ¹⁾	EX	248-315	(1.48±0.21)(10)	0	0	2
81 TRE/BAR ¹⁾	EX	238	(3.86±0.84)(10)			2
¹⁾ Stirred-flow reactor. Modulated molecular-beam Spectrometer. P(Total) = (1-3) torr.						
H + CO (+ M) → CHO (+ M)						
Hydrogen atom + Carbon monoxide						
78 GOR/IVA2 ¹⁾	EX	305	>1.51(10)			2
78 GOR/IVA2 ¹⁾	EX	375	>2.41(11)			2
¹⁾ Collision-induced shifts. HF-transition line broadening in H atoms. Lower-limit k's.						
71 BEN/BLA M = H ₂ . Upper-limit k.	EX	298	≤1.2(14)			3
71 HIK/EYR M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 1.54(H ₂).	EX	298	(2.6±0.4)(13)			3
72 AHU/MIC M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 1.0(He), 0.8(Ne), 1.1(Kr), 1.3(H ₂).	EX	298	(2.18±0.25)(15)			3
72 BAL/JAC M = H ₂ .	DE	773	2.3(14)			3
73 AZA/AND M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 2.0(CO).	EX	298	(3.99±2.18)(13)			3
80 HOC/SWO1 M = H ₂ . M-efficiencies relative to H ₂ are: 1.00(H ₂), 0.95(CO), 1.53(CH ₄). H ₂ Flash-photolysis in presence of CO. P = 760 torr.	EX	298	(3.8±0.4)(13)			3
H + CO + OH → HCHO + O						
Hydrogen atom + Carbon monoxide + Hydroxyl						
78 SME/PAV Shock-waves. Non-Arrhenius expression: ¹⁾ k = 4.35×10 ²⁰ (1/T) cm ⁶ mol ⁻² s ⁻¹	EX	1500-3500	¹⁾			3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
H + CO₂ → OH + CO						
Hydrogen atom + Carbon dioxide						
75 VAN/PEE k ₁ = k ₋₁ K.	DE	650-1800	4.8(14)	0	12582	2
78 WAW/ZIE H ₂ dissociation in a quartz vessel using the system ¹⁴ CO ₂ /CO/H ₂ . P(Total) = (100-200) torr.	EX	1013-1243	9.0(13)	0	12028	2
H + CH → H₂ + C						
Hydrogen atom + Methylidyne						
82 GRE/HOM2 Reaction of the Ethyne/O/H system, diluted in N ₂ /He, in a discharge-flow reactor. Resonance-fluorescence. O atoms generated by reacting N with NO. P = 2 torr.	EX	298	≈3.0(13)			2
H + CH₂ → H₂ + CH						
Hydrogen atom + Methylene						
82 GRE/HOM1 Reaction of the CH=CH/O/H system diluted in N ₂ /He, in a discharge-flow reactor. Resonance-fluorescence. O atoms generated by reacting N with NO. H atoms produced by a discharge of the mixture H ₂ /He. Best data fit. P = 2 torr.	EX	298	(5.0±1.0)(13)			2
H + CH₃ (+ M) → CH₄ (+ M)						
Hydrogen atom + Methyl						
72 TEN/JON Data-fit to a proposed mechanism.	CO	303-603	1.17(12)	0	25	2
74 CAM/MAR Average of three k's at 8, 12, and 16 torr., over the given T-range.	EX	503-753	(1.64±0.55)(12)	0	0	2
77 CHE/LEE	EX	308	1.5(14)			2
77 CHE/YEH Extrapolated limiting high-pressure k.	ES	308	(2.0±0.9)(14)			2
79 SEP/MAR ¹⁾ P(Ar) ~ 14 torr.	EX	750	2.82(12)			2
79 SEP/MAR ¹⁾ P(Ar) = 7.4 torr.	EX	768-818	1.58(12)			2
¹⁾ Discharge-flow system. Best data-fit.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 PAT/PIL Azomethane-Ethene flash-photolysis. Gas-chromatography. Limiting high-pressure k. M = Ar, or SF ₆ . P = (50-1000) torr.	EX	300	(9.03±4.22)(13)			2
80 SWO/HOC H ₂ O flash-photolysis. P ~760 torr. M = N ₂ , H ₂ .	EX	296	(1.2±0.3)(14)			2
74 PRA/VEL M = He. M-efficiencies relative to He are: 1.00(He), 37.74(NO).	EX	295	(5.3±1.0)(18)			3
76 PRA/VEL1 M = He. The preexponential factor expressed as: A(T/298) ^{-0.33} .	EX	321-521	1.06(19)	-0.33	0	3 5.01
H + CH₄ → H₂ + CH₃						
Hydrogen atom + Methane						
71 BAK/BAL Rate constant per CH bond.	CO	298-753	3.1(13)	0	5989	2
73 CLA/DOV1 BEBO calculation. The preexponential factor expressed as: A(T/298) ^{3.0} .	CO	300-1800	5.93(11)	3.0	4404±20	2 1.05
73 PEE/MAH1	EX	1600	(3.2±0.6)(12)			2
75 ROT/JUS	EX	1700-2300	7.23(14)	0	7578	2
78 SHA The preexponential factor expressed as: A(T/298) ² .	CO	300-2500	1.25(12)	2.0	4449	2
79 SEP/MAR ¹⁾ P(CH ₄) = (17-346) mtorr. P(Ar) = (5.2-14.8) torr.	EX	640-818	1.822(14)	0	6628±421	2 1.82
79 SEP/MAR ¹⁾ Extended T-range by combining the data of several workers. Recommended by author.	RE	400-1800	7.59(13)	0	6002±96	2 1.15
¹⁾ Discharge-flow system.						
80 ROT CH ₄ thermolysis behind shock-waves. Atomic Reso- nance-Absorption. Same data given in 79 ROT/JUS1.	EX	1800-2300	7.23(14)	0	7600	2
80 MUR/BOR1 ²⁾	RL	1550	8.0(-1)			2/2
80 MUR/BOR1 ²⁾	RL	1923	1.46			2/2
²⁾ Oxidative pyrolysis of CH ₄ behind reflected shock-waves, initiated by the N ₂ O decomposition. Within the T-range (1550-1923) K, the ratio of rate constants shows a trend to increase from about 0.7 to 1.5. k _{ref} : N ₂ O + M → N ₂ + O + M.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
D + CD₄ → D₂ + CD₃						
Deuterium atom + Methane-d ₄						
80 CHI/BAK CD ₄ Pyrolysis behind shock-waves. Resonance-absorption Spectroscopy.	EX	1780-2440	2.1(15)	0	11223	2
H + CHO → H₂ + CO (a)						
→ HCHO (b)						
→ O + CH ₂ (c)						
Hydrogen atom + Methyl, oxo-						
73 MAC/THR k _a /k _{ref} . k _{ref} : CHO + O → CO + OH (m) → CO ₂ + H (n)	RL	300	4.0			2/2
78 REI/CLA k _a . HCHO photolysis with tunable pulsed UV laser.	EX	298	3.31(14)			2 2.0
79 NAD/SAR4 k _a . Intracavity laser spectroscopy. Unreported T assumed to be 298 K. Lower-limit k.	EX	298	>3.01(13)			2
81 CHE/RHO k _a . Kinetic modelling of CO oxidation in flames.	ES	250-2000	(4.0±1.0)(13)			2
78 NAD/SAR ¹⁾ k(a + b)/k _{ref} . k _{ref} : CHO + CHO → products.	RL	298	(6.7±2.7)			2/2
78 NAD/SAR ¹⁾ k(a + b). ¹⁾ HCHO Flash-photolysis. Laser-spectroscopy.	RN	298	1.45(14)			2
79 NAD/SAR2 k _a + k _b . Pulse-photolysis of CH ₃ CHO.	EX	298	(1.20±0.42)(14)			2
80 HOC/SW01 k _a + k _b . H ₂ flash-photolysis in presence of CO. P = 760 torr.	EX	298	(6.9±1.7)(13)			2
81 TSU/KAT ²⁾ Total conc. = 6.0x10 ¹⁸ molec.cm ⁻³ .	RN	1500-1900	1.28(10)	0	-2285	2
81 TSU/KAT ²⁾ Total conc. = 3.0x10 ¹⁹ molec.cm ⁻³ .	RN	1500-1900	4.68(10)	0	-2285	2
81 TSU/KAT ²⁾ Total conc. = 6.0x10 ¹⁹ molec.cm ⁻³ .	DE	1500-1900	6.61(10)	0	-2285	2
²⁾ k _b . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ in Ar behind reflected shock-waves. UV-absorption. IR-emission. k ₁ ~ k ₋₁ K.						
81 TSU/HAS k _c . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ in Ar behind reflected shock-waves.	ES	1200-1800	3.98(13)	0	51602	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
H + HCHO → H₂ + CHO (a)						
→ CH₂OH (b)						
Hydrogen atom + Formaldehyde						
72 RID/DAV k _a .	EX	297	(3.25±0.30)(10)			2
72 WES/DEH2 k _a .	EX	297-652	1.35(13)	0	1892	2
77 SLE/WAR k _a .	EX	298	(2.59±1.81)(10)			2
78 NAD/SAR k _a . HCHO Flash-photolysis. Laser-spectroscopy.	EX	298	(1.81±0.78)(10)			2
79 KLE k _a . Flash-photolysis. Resonance-fluorescence. Mass-spectrometry.	EX	250-500	(1.97±0.97)(13)	0	1847±184	2
80 DEA/JOH1 k _a . HCHO Decomposition behind shock-waves. Best data-fit. Total conc. = 5x10 ¹⁸ molec.cm ⁻³ .	EX	1700-2500	3.31(14)	0	5281	2
81 TSU/KAT ¹⁾ Total conc. = 6.0x10 ¹⁸ molec.cm ⁻³ .	ES	1200-1800	2.95(9)	0	601	2
81 TSU/KAT ¹⁾ Total conc. = 3.0x10 ¹⁹ molec.cm ⁻³ .	ES	1200-1800	1.26(10)	0	601	2
81 TSU/KAT ¹⁾ Total conc. = 6.0x10 ¹⁹ molec.cm ⁻³ .	DE	1200-1800	2.34(10)	0	601	2
¹⁾ k _b . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ mixtures diluted in Ar behind reflected shock- waves. UV-absorption. IR-emission. k ₁ = Kk ₋₁ . Same data given in 81 TSU/HAS.						
H + CH₃O → H₂ + HCHO (a)						
→ OH + CH₃ (b)						
Hydrogen atom + Methoxy						
77 MOO/SLE k _a /(k _a + k _b). Most probable ratio.	RL	223-398	(3.1±3.0)(-1)			2/2
77 MOO/SLE k _b /(k _a + k _b). Most probable ratio.	RL	223-398	(6.9±3.0)(-1)			2/2
81 HOY/LOF ¹⁾ (k _a + k _b)/k _{ref} . k _{ref} : H + CH ₂ OH → products.	RL	300	6.7(-1)			2/2
81 HOY/LOF ¹⁾ k _a + k _b .	RN	300	2.0(13)			2
¹⁾ Discharge-flow. Laval nozzle. Mass-spectrometry. Channel (a) the major path. P = (0.1-2.0) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
H + CD₃O → HD + HCHO (a)							
→ OH + CD₃ (b)							
Hydrogen atom + Methoxy-d ₃							
81 HOY/LOF ¹⁾ (k _a + k _b)/k _{ref} . k _{ref} : H + CD ₂ OH → products.	RL	300	(6.8±1.9)(-1)				2/2
81 HOY/LOF ¹⁾ k _a + k _b .	RN	300	1.9(13)				2
¹⁾ Discharge fast flow-reactor. Laval nozzle reactor. Mass-spectrometry. Channel (a) is the major path. P = (0.1-2.0) torr.							
D + CH₃O → HD + HCHO (a)							
→ OD + CH₃ (b)							
Deuterium atom + Methoxy							
81 HOY/LOF ¹⁾ (k _a + k _b)/k _{ref} . k _{ref} : D + CH ₂ OD → products.	RL	300	7.1(-1)				2/2
81 HOY/LOF ¹⁾ k _a + k _b .	RN	300	2.2(13)				2
¹⁾ Discharge fast flow-reactor. Laval nozzle reactor. Mass-spectrometry. Channel (a) is the major path. P = (0.1-2.0) torr.							
H + CH₂OH → H₂ + HCHO (a)							
→ OH + CH₃ (b)							
Hydrogen atom + Methyl, hydroxy-							
81 HOY/LOF k _a + k _b . Discharge fast-flow reactor. Laval nozzle reactor. Mass-spectrometry. Channel (a) is the major path. P = (0.1-2.0) torr.	RN	300	3.0(13)				2
H + CD₂OH → H₂ + DCDO (a)							
→ HD + HCDO (b)							
→ OH + CD₂H (c)							
Hydrogen atom + Methyl-d ₂ , hydroxy-							
81 HOY/LOF k _a + k _b + k _c . Discharge fast flow-reactor. Laval nozzle reactor. Mass-spectrometry. Channels (a) and (b) are major. P = (0.1-2.0) torr.	RN	300	2.9(13)				2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref)), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
D + CH ₂ OD → D ₂ + HCHO (a)						
→ DH + HCDO (b)						
→ OD + CH ₂ D (c)						
Deuterium atom + Methyl, hydroxy-d						
81 HOY/LOF	RN	300	3.2(13)			2
k _a + k _b + k _c .						
Discharge fast flow-reactor. Laval						
Laval nozzle reactor. Mass-spectrometry.						
Channels (a) and (b) are major.						
P = (0.1-2.0) torr.						
H + CH ₃ OH → H ₂ O + CH ₃ (a)						
→ H ₂ + CH ₂ OH (b)						
→ OH + CH ₄ (c)						
→ H ₂ + CH ₃ O (d)						
Hydrogen atom + Methanol						
71 ADE/WAG	EX	295-653	(2.3±0.2)(13)	0	2667±151	2
k _a + k _b + k _c + k _d .						
73 ADE	EX	298-650	1.3(13)	0	2670	2
k _a + k _b .						
74 MEA/KIM	EX	298-565	(1.80±0.33)(12)	0	2738±65	2
k _b . Flow-discharge method with ESR detection.						
74 MEA/KIM	RE	298-575	6.5(12)	0	2738±75	2
k _b . Assumed A-factor on the basis of						
stoichiometric considerations.						
Recommended k.						
81 HOY/SIE	EX	500-680	1.3(13)	0	2646	2
k _b + k _d . Isothermal discharge-flow reactor.						
Mass-spectrometry.						
P = (1.5-6) torr.						
81 VAN/VAN	DE	1000-2000	3.4(13)	0	1309	2
k _b . Methanol oxidation in lean flames.						
CH ₃ OH/O ₂ mixtures, with or without added						
Ar or H ₂ , burned at 40 torr.						
Molecular beam sampling. Mass-spectrometry.						
H + CD ₃ OH → H ₂ + CD ₃ O (a)						
→ HD + CD ₂ OH (b)						
Hydrogen atom + Methan-d ₃ -ol						
81 HOY/SIE	EX	500-680	1.3(13)	0	2646	2
k _a + k _b . Isothermal discharge-flow reactor.						
Mass-spectrometry.						
P = (1.5-6) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$H + CD_3OD \rightarrow HD + CD_3O$ (a) $\rightarrow HD + CD_2OD$ (b) Hydrogen atom + Methanol-d ₄						
81 HOY/SIE $k_a + k_b$. Discharge-flow. P = (1.5-6) torr.	EX	500-680	1.3(13)	0	2646	2
$D + CH_3OH \rightarrow DH + CH_3O$ (a) $\rightarrow DH + CH_2OH$ (b) Deuterium atom + Methanol						
81 HOY/SIE $k_a + k_b$. Discharge-flow. P = (1.5-6) torr.	EX	500-680	1.3(13)	0	2646	2
74 MEA/KIM k_b . Discharge-flow with ESR detection.	ES	298-575	(2.82±0.40)(13)	0	2617±50	2
$H + CH_3OOH \rightarrow H_2O + CH_3O$ (a) $\rightarrow H_2 + CH_3O_2$ (b) $\rightarrow H_2 + CH_2OOH$ (c) Hydrogen atom + Hydroperoxide, methyl-						
75 SLE/WAR2 $k_a + k_b + k_c$.	EX	250-358	(1.69±0.54)(11)	0	956±101	2
77 SLE/WAR $k_a = (43±7)\%$ of k(overall).	EX	250-358	(7.27±0.18)(10)	0	936±96	2
77 SLE/WAR $k_b = (52±7)\%$ of k(overall).	EX	250-358	(8.79±0.18)(10)	0	936±96	2
77 SLE/WAR $k_c = 5\%$ of k(overall).	EX	250-358	8.45(9)	0	936±96	2
77 SLE/WAR ¹⁾	EX	250-358	(1.69±0.54)(11)	0	936±96	2
77 SLE/WAR ¹⁾ ¹⁾ $k_a + k_b + k_c$.	EX	298	(7.83±1.20)(9)			2
$D + CH_3OOH \rightarrow DHO + CH_3O$ (a) $\rightarrow DH + CH_3O_2$ (b) $\rightarrow DH + CH_2OOH$ (c) Deuterium atom + Hydroperoxide, methyl-						
77 SLE/WAR $k_a + k_b + k_c$.	EX	298	(7.23±0.60)(9)			2
$H + COS \rightarrow SH + CO$ Hydrogen atom + Carbon oxide sulfide						
72 ROM/SCH	EX	298	(1.33±0.24)(10)			2
75 TSU/YOK	EX	300-525	(9.1±1.2)(12)	0	1963±186	2
76 LEE	EX	298-478	(9.77±1.00)(13)	0	2774±39	2
77 LEE/STI	EX	261-500	(5.46±0.92)(12)	0	1938±55	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$H + CH_2=N=N \rightarrow CH_3 + N_2$ Hydrogen atom + Methane, diazo-						
72 NIK/MOR2	EX	300	9.64(12)			2
$H + CH_3NO_2 \rightarrow \text{products}$ Hydrogen atom + Methane, nitro-						
75 SLE/WAR2	EX	298-398	(1.63±0.60)(12)	0	1761±126	2
$H + CH_3ONO \rightarrow NO + CH_3OH$ (a) → $H_2 + CH_2ONO$ (b) → $HNO + CH_3O$ (c) Hydrogen atom + Nitrous acid methyl ester (Methyl nitrite)						
77 MOO/SLE $k_a = (47\pm5)\%$ of k(overall).	EX	223-398	(1.21±0.13)(11)	0	956±55	2
77 MOO/SLE $k_b + k_c = (53\pm5)\%$ of k(overall).	EX	223-398	(1.37±0.13)(11)	0	956±55	2
77 MOO/SLE $k_a + k_b + k_c$.	EX	223-398	(2.58±0.51)(11)	0	956±55	2
$H + CD_3ONO \rightarrow NO + CD_3OH$ (a) → $HD + CH_2ONO$ (b) → $HNO + CD_3O$ (c) Hydrogen atom + Nitrous acid methyl-d ₃ ester (Methyl-d ₃ nitrite)						
77 MOO/SLE $k_a + k_b + k_c$.	EX	298	(8.31±1.39)(9)			2
$H + CH\equiv CH (+ M) \rightarrow H_2 + CH\equiv C (+ M)$ (a) → $CH_2=CH (+ M)$ (b) Hydrogen atom + Ethyne						
74 YAM/LAV k_a .	EX	1063-1233	4.78(13)	0	8254±2013	2 2.51
71 OSB ¹⁾	EX	298	2.71(10)			2
75 IBU/TAK ¹⁾ ¹⁾ k_b .	EX	296	(5.5±0.5)(10)			2
76 KEI/LYN ²⁾ k increasing from (6.32±0.60)×10 ⁹ to (1.29±0.12)×10 ¹⁰ cm ³ mol ⁻¹ s ⁻¹ within the (1-10) torr. P-range. Low P-range. $k_b = k_{app}/s$, where s ~ 2.0.	EX	298	(6.32±0.60)(9)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 KEI/LYN ²) k increasing from $(2.37 \pm 0.26) \times 10^{10}$ to $(9.43 \pm 0.58) \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ within the (6-742) torr. P-range. High P-range. $k_{bi} = k_{app}/s$, where $s \sim 1.15$.	EX	298	$(2.37 \pm 0.86)(10)$			2
²) k_b . Initial step in a proposed mechanism. Addition product vibrationally excited. P-dependent k's.						
76 PAY/STI k_b . M = He. Limiting high-pressure k. Initial step in a proposed mechanism.	EX	193-400	$(5.54 \pm 1.57)(12)$	0	1213 $\pm$ 70	2
78 GOR/IVA2 ³) Method based on collision-induced shifts and HF-transition line broadening in H atoms.	EX	305	$(2.11 \pm 0.18)(11)$			2
78 GOR/IVA2 ³) Method based on H-maser relaxation.	EX	305	$(2.11 \pm 0.12)(11)$			2
78 GOR/IVA2 ³) Method based on collision-induced shifts and HF-transition line broadening in H atoms.	EX	305	$(9.43 \pm 3.63)(16)$			3
³) k_b .						
79 ISH/SUG2 k_b . Pulse-radiolysis. Absorption-Spectroscopy. P = (200-1100) torr. H + 0.073 torr. CH=CH.	EX	298	$(2.29 \pm 0.24)(11)$			2
81 SUG/OKA2 k_b . Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k.	EX	206-461	$(2.28 \pm 0.12)(13)$	0	1374 $\pm$ 18	2
H + CD=CD (+ M) $\rightarrow$ D + CH=CD (+ M) (a) $\rightarrow$ CHD=CD (+ M) (b)						
Hydrogen atom + Ethyne-d ₂						
71 HOY/WAG k_a .	EX	300-470	2.0(13)	0	2667 $\pm$ 252	2
76 KEI/LYN ¹) k increasing from $(3.98 \pm 0.42) \times 10^{10}$ to $(5.84 \pm 0.60) \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ within the (1.2-5.6) torr. pressure range. Experiments in excess [CD=CD].	EX	298	$(3.98 \pm 0.42)(10)$			2
76 KEI/LYN ¹) k increasing from $(2.11 \pm 0.24) \times 10^{10}$ to $(3.49 \pm 0.36) \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ within the (1-5) torr. pressure range. Experiments in excess [H].	EX	298	$(2.11 \pm 0.24)(10)$			2
¹) k_a . Overall reaction of a proposed mechanism. P-dependent rate constants.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
78 GOR/IVA2 ²⁾	EX	305	(2.35±0.48)(11)			2
78 GOR/IVA2 ²⁾	EX	305	(9.98±5.44)(16)			3
²⁾ k _b . Collision-induced shifts. HF-transition line broadening in H atoms.						
79 ISH/SUG2	EX	298	(2.29±0.12)(11)			2
k _b . Pulse-radiolysis. Absorption-spectroscopy. P = (200-1100) torr. (H ₂ + CD≡CD)						
81 SUG/OKA2	EX	206-461	(1.91±0.12)(13)	0	1330±24	2
k _b . Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k.						
D + CH≡CH → H + CH≡CD (a) → CHD=CH (b)						
Deuterium atom + Ethyne						
71 HOY/WAG	EX	200-465	3.1(13)	0	1862±101	2
k _a .						
76 KEI/LYN	EX	298	(7.35±0.72)(10)			2
k _a . Overall reaction of a proposed mechanism. Average k for the pressure range (1-6.7) torr.						
79 ISH/SUG2	EX	298	(1.57±0.12)(11)			2
k _b . Pulse-radiolysis. Absorption-spectroscopy. P = (200-1100) torr. (D ₂ + CH≡CH)						
81 SUG/OKA2	EX	206-461	(2.07±0.37)(13)	0	1521±59	2
k _b . Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k.						
D + CD≡CD → CD ₂ =CD						
Deuterium atom + Ethyne-d ₂						
76 KEI/LYN	EX	298	(6.63±0.60)(9)			2
k increasing from (6.63±0.60)×10 ⁹ to (1.08±0.12)×10 ¹⁰ cm ³ mol ⁻¹ s ⁻¹ within the (1-5 6) torr. P-range. P-dependent k. k _{bi} = k _{app} /s, where s ~ 2.0. The addition product is vibrationally excited.						
79 ISH/SUG2	EX	298	(1.51±0.12)(11)			2
Pulse-radiolysis. Absorption-spectroscopy. P = (200-1100) torr. (D ₂ + CD≡CD)						
81 SUG/OKA2	EX	206-461	(2.64±0.87)(13)	0	1602±18	2
Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
H + CH₂=CH → H₂ + CH=CH						
Hydrogen atom + Ethenyl						
80 TAN/GAR1	ES	2000-2450	1.0(13)	0	0	2
Thermolysis of CH ₂ =CH ₂ in Ar behind incident shock-waves. Optimization.						
Total conc. = (1.1-2.2)×10 ¹⁸ molec.cm ⁻³ .						
H + CH₂=CH₂ (+ M) → H₂ + CH₂=CH (+ M) (a)						
→ CH ₃ CH ₂ (+ M) (b)						
Hydrogen atom + Ethene						
72 FAL/SUN	RL	298	≤3.0(-4)			2/2
k _a /k _b . Upper-limit ratio.						
73 PEE/MAH2 ¹⁾	ES	1200-1700	1.1(14)	0	4278	2
74 YAM2 ¹⁾	EX	1093-1213	1.91(13)	0	5184±1007	2 2.51
75 NAM/SHE ¹⁾	EX	1073-1173	(1.5±0.4)(11)			2
75 NAM/SHE ¹⁾	ES	1073-1173	8.47(12)	0	4529±201	2
A-factor recalculated from the author's estimated value for E _a .						
77 JUS/ROT ¹⁾	ES	1700	5.0(12)			2
77 JUS/ROT ¹⁾	ES	2000	1.5(13)			2
77 JUS/ROT ¹⁾	ES	1700-2000	5.0(15)	0	11500	2
81 HAU/SAN ¹⁾	EX	1110-1235	3.54(14)	0	7217	2
Propane pyrolysis. Adiabatic flow-reactor.						
¹⁾ k _a .						
71 COW/KEI ²⁾	RL	298	(8.6±1.3)			2/2
k _b /k _{ref} .						
k _{ref} : H + CH=CH → CH ₂ =CH [†]						
71 COW/KEI ²⁾	RN	298	(2.35±0.60)(11)			2
k _b .						
²⁾ M = Ne, Ar. Steady-state photolysis method.						
The addition product is vibrationally excited.						
P(Total) = (10-15) torr.						
71 HIK/EYR	EX	298	(5.5±0.5)(11)			2
k _b . M = H ₂ , or Ar. Limiting high-pressure k.						
The addition product is vibrationally excited.						
71 OSB	EX	298	3.70(11)			2
k _b .						
71 PEN/DAR ³⁾	RL	303-478	3.0(-1)	0	425	2/2
k _b /k _{ref} .						
k _{ref} : H + HI → H ₂ + I.						
71 PEN/DAR ³⁾	RN	298	(6.9±0.7)(11)			2
k _b .						
³⁾ Photolysis of HI in presence of Ethene.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
72 TEN/JON k _b . Data-fit to a proposed mechanism.	CO	303-603	7.89(11)	0	367	2
73 MIC/OSB k _b . M = He. Limiting high-pressure k.	EX	298	(9.70±0.19)(11)			2
74 LAU/BUE ⁴⁾ k _{ref} : H + CH ₃ CH=CH ₂ → (CH ₃) ₂ CH [†]	RL	298	(5.6±0.2)(-1)			2/2
74 LAU/BUE ⁴⁾ k _{ref} : H + CH ₃ CH=CHCH ₃ → CH ₃ CH ₂ CHCH ₃ [†]	RL	298	(1.2±0.2)			2/2
74 LAU/BUE ⁴⁾ k _{ref} : H + (CH ₃) ₂ C=CHCH ₃ → (CH ₃) ₂ CCH ₂ CH ₃ [†] (c) → (CH ₃) ₂ CHCHCH ₃ [†] (d)	RL	298	(8.0±2.0)(-1)			2/2
⁴⁾ k _b /k _{ref} . The product is vibrationally excited.						
74 LAU/BUE k _b . The product is vibrationally excited.	EX	298	2.47(11)			2
75 IBU/TAK k _b /k _{ref} . Conventional vacuum apparatus. k _{ref} : H + CH≡CH → CH ₂ =CH	RL	296	9.99±0.16			2/2
75 MIH/SCH k _b . The product is vibrationally excited.	EX	295	(7.53±0.24)(11)			2
78 GOR/IVA2 k _b . Method based on collision-induced shifts and HF-transition line broadening in H atoms.	EX	305	(6.32±0.60)(11)			2
78 GOR/IVA2 k _b . Method based on H-maser relaxation.	EX	305	(6.63±0.12)(11)			2
78 GOR/IVA2 k _b . Method based on collision-induced shifts and HF-transition line broadening in H atoms.	EX	305	(4.35±1.45)(17)			3
78 ISH/YAM k _b . Pulse-radiolysis. Resonance-absorption. P(H ₂) = (200-1200) torr.	EX	298	(6.63±0.60)(11)			2
78 LEE/MIC1 k _b . M = Ar. Flash-photolysis. Resonance- fluorescence. P(CH ₂ =CH ₂) = (13-150) torr. P(Ar) = (300-760) torr.	EX	198-320	(2.21±0.40)(13)	0	1040±42	2
79 OKA/CVE ⁵⁾ k _b /k _{ref} . k _{ref} : H + NO + M → HNO + M.	RL	298	(3.41±0.06)(-2)			2/3
79 OKA/CVE ⁵⁾ k _b .	RN	298	(4.69±0.15)(11)			2
⁵⁾ Modulated Hg-photosensitization. Chemilumines- cence. k is P-dependent, decreasing with lower P-values. The product is vibrationally excited. P = 100 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 BIL/BAR k_b . Ethane pyrolysis. k determined relative to the reaction: $H + CH_3CH_3 \rightarrow H_2 + CH_3CH_2$	RN	793-829	3.98(13)	0	2345	2
81 EKW/SAF2 k_b/k_{ref} . H atoms generated by Hg-photosensitized decomposition of H_2 . General vacuum apparatus. Gas-chromatography. $P(H_2) \sim 580$ torr. $P(\text{Diethylsulfide}) = (1-32)$ torr. k_{ref} : $H + (CH_3CH_2)_2S \rightarrow CH_3CH_2SH + CH_3CH_2$	RL	358-461	4.66(-1)	0	-871±35	2/2
81 SUG/OKA2 k_b . Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k. Supersedes 81 SUG/OKA1.	EX	206-461	(2.83±0.30)(13)	0	1096±29	2
$H + CH_2=CHD \rightarrow CH_3CHD$ (a) $\rightarrow CH_2DCH_2$ (b) Hydrogen atom + Ethene-d						
81 SUG/OKA2 $k_a + k_b$. Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k. Supersedes 81 SUG/OKA1.	EX	206-461	(2.67±0.46)(13)	0	1084±50	2
$H + CD_2=CD_2 (+M) \rightarrow D + CD_2=CDH (+M)$ (a) $\rightarrow CD_2HCD_2 (+M)$ (b) Hydrogen atom + Ethene-d ₄						
74 YAM1 k_a . Averaged over the given T-range.	EX	1000-1200	6.75(12)			2 1.35
71 OSB k_b .	EX	298	5.44(11)			2
71 PEN/DAR ¹⁾ k_b/k_{ref} . k_{ref} : $H + HI \rightarrow H_2 + I$.	RL	303-478	3.0(-1)	0	425	2/2
71 PEN/DAR ¹⁾ k_b .	RN	298	(7.6±0.8)(11)			2
¹⁾ Photolysis of HI in presence of $CD_2=CD_2$.						
75 COW/MIC k_b . In excess H, at 0.91rr. k increasing to $5.90 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 4.93 torr.	EX	297	4.16(11)			2
75 MIH/SCH k_b . The product is vibrationally excited.	EX	295	(6.93±0.24)(11)			2
78 GOR/IVA2 k_b . Collision-induced shifts. HF-transition line broadening in H atoms.	EX	305	(6.99±0.48)(11)			2
78 GOR/IVA2 k_b . Method based on H-maser relaxation.	EX	305	(6.02±0.12)(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
78 GOR/IVA2 k_b . Collision-induced shifts. HF-transition line broadening in H atoms.	EX	305	(3.63±1.09)(17)			3
81 SUG/OKA2 k_b . Pulse-radiolysis. Resonance-absorption. Li- miting high-pressure k. Supersedes 81 SUG/OKA1.	EX	206-461	(2.75±0.30)(13)	0	1087±26	2
$+ CH_2=CH_2 \rightarrow CDH_2CH_2$						
Deuterium atom + Ethene						
75 COW/MIC In excess D. P-independent from 0.96 to 5 torr.	EX	297	(4.60±0.04)(11)			2
75 COW/MIC In excess $CH_2=CH_2$. Relatively stable k from 1.25 to 1.76 torr., but increasing to $7.29 \times 10^{11} \text{ cm}_3 \text{ mol}^{-1} \text{ s}^{-1}$ at 4.16 torr.	EX	297	(4.68±0.34)(11)			2
75 MIH/SCH The product is vibrationally excited.	EX	295	(5.24±0.18)(11)			2
79 ISH/SAT Pulse-radiolysis. Resonance-absorption.	EX	298	(4.82±0.60)(11)			2
81 SUG/OKA2 Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k. Supersedes 81 SUG/OKA1.	EX	206-461	(2.02±0.09)(13)	0	1100±12	2
$D + CH_2=CHD \rightarrow CDH_2CHD$ (a)						
$\rightarrow CD_2HCH_2$ (b)						
Deuterium atom + Ethene-d						
81 SUG/OKA2 $k_a + k_b$. Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k. Supersedes 81 SUG/OKA1.	EX	206-461	(2.15±0.20)(13)	0	1104±28	2
$D + CD_2=CD_2 \rightarrow CD_3CD_2$						
Deuterium atom + Ethene-d ₄						
71 OSB	EX	298	4.37(11)			2
75 COW/MIC In excess D, at 0.95 torr. k increasing to $2.77 \times 10^{11} \text{ cm}_3 \text{ mol}^{-1} \text{ s}^{-1}$ at 5 torr.	EX	297	1.33(11)			2
75 MIH/SCH The product is vibrationally excited.	EX	295	(5.12±0.30)(11)			2
81 SUG/OKA2 Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k. Supersedes 81 SUG/OKA1.	EX	206-461	(2.14±0.26)(13)	0	1115±36	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
H + CH₃CH₂ → CH₃ + CH₃ (a)						
→ H₂ + CH₂=CH₂ (b)						
Hydrogen atom + Ethyl						
72 TEN/JON ¹⁾	DE	303-603	1.08(14)	0	438	2
Data-fit to a proposed mechanism.						
74 CAM/MAR ¹⁾	EX	503-753	3.72(13)	0	0	2
74 PRA/VEL ¹⁾	EX	295	(4.3±0.4)(13)			2
76 PRA/VEL ¹⁾	EX	321-521	6.46(13)	0	112±35	2 1.12
79 TAB/BAU ¹⁾	EX	1950-2770	1.0(13)	0	0	2
M = Ar. CH ₄ pyrolysis in shock-waves.						
Best data-fit.						
Total conc. = (1.4-5.4)×10 ¹⁸ molec.cm ⁻³ .						
¹⁾ k _a .						
74 CAM/MAR	EX	503-753	1.70(12)	0	0	2
k _b .						
H + CH₃CH₃ → H₂ + CH₃CH₂						
Hydrogen atom + Ethane						
71 BAK/BAL	CO	298-753	2.2(13)	0	4882	2
Rate constant per CH bond.						
72 KAL/KOR	ES	1073-1173	(3.31±2.71)(12)	0	0	2
Average of two given values.						
73 CLA/DOV1	CO	300-1800	2.45(11)	3.5	2617±35	2 1.07
BEBO calculation. The preexponential factor expressed as: A(T/298) ^{3.5} .						
74 CAM/MAR	SE	290-1290	1.32(14)	0	4715±108	2 1.23
74 CAM/MAR	EX	503-753	1.86(14)	0	4920±192	2 1.35
74 KAL/SHE	EX	1023-1123	(2.4±0.6)(12)			2
77 JON/MOR	EX	357-544	1.07(14)	0	4642±313	2 1.86
Discharge-flow. Mass-spectrotry.						
78 LED/VIL	EX	281-1485	5.01(13)	0	4580±302	2 3.98
Discharge-flow reactor.						
79 BAL/WAL1	CO	753-773	1.32(14)	0	4715	2
A and B recalculated from an empirical formula.						
H + CH₂=C=O → CH₃ + CO						
Hydrogen atom + Ethenone (Ketene)						
75 SLE/WAR1	EX	218-363	(3.61±1.20)(12)	0	1178±101	2
75 SLE/WAR1	EX	300	(7.23±0.60)(10)			2
79 MIC/NAV1 ¹⁾	EX	298-500	(1.13±0.67)(13)	0	1725±190	2
79 MIC/NAV1 ¹⁾	EX	298	(3.73±1.01)(10)			2
79 MIC/NAV1 ¹⁾	EX	298	(4.40±0.78)(10)			2
¹⁾ Flash-photolysis. Discharge-flow.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{H} + \text{CH}_3\text{CO} \rightarrow \text{H}_2 + \text{CH}_2=\text{C}=\text{O}$ (a) $\rightarrow \text{CHO} + \text{CH}_3$ (b)						
Ethyl, 1-oxo- + Hydrogen atom						
75 SLE/WAR1 $k_a/(k_a + k_b)$.	RL	298	(6.3±0.7)(-1)			2/2
75 SLE/WAR1 $k_b/(k_a + k_b)$.	RL	298	3.7(-1)			2/2
$\text{H} + \text{CH}_3\text{CHO} \rightarrow \text{H}_2 + \text{CH}_3\text{CO}$						
Hydrogen atom + Acetaldehyde						
73 ADE/WAG1	EX	295-389	(2.6±0.2)	0	1309±75	2
75 SLE/WAR1 $k_{\text{ref}}: \text{H} + \text{CH}_2=\text{C}=\text{O} \rightarrow \text{CO} + \text{CH}_3$	RL	298	(4.6±0.2)(-1)			2/2
75 SLE/WAR1	RN	298	3.19(10)			2
76 WHY/MIC2	EX	298-500	(1.34±0.23)(13)	0	1661±60	2
77 MIC/LEE Discharge-flow. Resonance-fluorescence.	EX	298	(5.90±0.48)(10)			2
$\text{H} + \text{CH}_2\text{CH}_2\text{OH} \rightarrow \text{H} + [\text{C}_2\text{H}_4\text{O}]$						
Hydrogen atom + Ethyl, 2-hydroxy-						
82 BAR/HOY Discharge-flow. Laval-nozzle. P < 0.2 torr.	EX	~295	≈5.0(13)			2
$\text{H} + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{H}_2 + \text{CH}_3\text{CHOH}$ (a) $\rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}_2$ (b)						
Hydrogen atom + Ethanol						
73 ADE/WAG2 k_a .	EX	295-700	≈4.4(12)	0	2300	2
73 ADE/WAG2 k_b .	EX	295-700	≈5.9(11)	0	1736	2
73 ADE ¹⁾	EX	298-470	4.2(12)	0	2117	2
73 ADE/WAG2 ¹⁾	EX	295-700	(4.2±0.4)(12)	0	2115±150	2
¹⁾ $k_a + k_b$.						
$\text{H} + (\text{CH}_3)_2\text{O} \rightarrow \text{H}_2 + \text{CH}_3\text{OCH}_2$						
Hydrogen atom + Methane, oxybis-						
74 MEA/KIM ¹⁾ Electron-Spin-Resonance measurements.	EX	300-404	(2.61±0.13)(13)	0	2365±25	2
74 MEA/KIM ¹⁾ Mass-spectrometric measurements, assumed free from stoichiometric factors.	EX	300-404	(1.3±0.5)	0	2365±50	2
¹⁾ Flow-discharge method.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
77 SLE/WAR	EX	298	(7.83±2.41)(8)			2
78 ARO ²⁾	ES	1062	2.0(12)			2
78 ARO ²⁾	ES	1223	2.0(13)			2
²⁾ Pyrolysis in a flow-reactor.						
78 LEE/MAC Flash-photolysis. Resonance-fluorescence.	EX	273-426	(2.64±0.36)(12)	0	1956±43	2
79 FAU/HOY Discharge-flow. Mass-spectrometry.	EX	250-620	(1.9±0.9)(13)	0	2600±100	2
81 LEE/MAC Flash-photolysis. Resonance-fluorescence. [(CH ₃) ₂ O] ₀ ~1.0x10 ¹⁶ molec.cm ⁻³ . [H] ₀ <1.0x10 ¹¹ molec.cm ⁻³ .	EX	273-426	(2.64±0.36)(12)	0	1956±43	2
D + (CH ₃) ₂ O → DH + CH ₃ OCH ₂ Deuterium atom + Methane, oxybis-						
74 MEA/KIM Flow-discharge method with ESR detection.	EX	198-363	(4.14±0.73)(13)	0	2229±50	2
H + CH ₃ OOCH ₃ → H ₂ + CH ₂ OOCH ₃ Hydrogen atom + Peroxide, dimethyl-						
77 SLE/WAR	EX	298	(7.23±0.60)(8)			2
H + Δ → SH + CH ₂ =CH ₂ Hydrogen atom + Thiirane (Ethylene episulfide)						
75 YOK/AHM	RN	300-425	(5.7±0.7)(13)	0	978±88	2
76 LEE	EX	298	(7.10±1.08)(11)			2
77 LEE/STI	EX	223-423	(1.73±0.07)(13)	0	946±12	2
H + (CH ₃) ₂ S → H ₂ + CH ₃ SCH ₂ (a) → CH ₃ + CH ₃ SH (b) Hydrogen atom + Methane, thiobis-						
76 LEE k _a + k _b .	EX	300	(9.0±3.0)(10)			2
81 LEE/MAC ¹⁾	EX	212-500	(7.83±2.59)(12)	0	1118±81	2
81 LEE/MAC ¹⁾	EX	212-298	(2.60±0.36)(12)	0	853±23	2
81 LEE/MAC ¹⁾	EX	298-500	(1.51±0.04)(13)	0	1372±9	2
¹⁾ k _a . Flash-photolysis. Resonance-fluorescence. Gas-chromatography. Arrhenius plot seems curved over the whole whole T-range of (212-500) K. [(CH ₃) ₂ S] ₀ ~1.0x10 ¹⁴ molec.cm ⁻³ . [H] ₀ <1.0x10 ¹¹ molec.cm ⁻³ .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 YOK/STR k_b . H atoms generated by H_2S photolysis in excess He, or CO_2 . General-vacuum system. P = 760 torr.	EX	300-472	(1.71±0.26)(13)	0	1319±44	2
$H + CH_3SSCH_3 \rightarrow CH_3SH + CH_3S$ Hydrogen atom + Disulfide, dimethyl-						
80 EKW/JOD Hg-sensitized reaction. $P(H_2) = (570-590)$ torr.	EX	298-428	(5.7±1.2)(12)	0	50±50	2
$H + NCCN \rightarrow HCN + CN$ (a) $\rightarrow HC_2N_2^\dagger$ (b) Hydrogen atom + Ethanedinitrile						
71 DUN/FRE k_a . P(Total) ~ 1 torr.	EX	298	(5.18±1.81)(8)			2
78 PHI k_b . Discharge-flow. Resonance-fluorescence. High-pressure k.	EX	300	(9.03±1.20)(8)			2
$H + O=C=C=O \rightarrow CO + OC=CH$ Hydrogen atom + 1,2-Propadiene-1,3-dione						
77 FAU/WAG1	EX	295-480	(1.7±0.6)(13)	0	1480±180	2
$H + CH_3C\equiv CH \rightarrow CH_3C=CH_2^\dagger$ (a) $\rightarrow CH_3CH=CH^\dagger \rightarrow CH_3 + CH\equiv CH$ (b) Hydrogen atom + 1-Propyne						
72 WAG/ZEL2 k_a .	EX	195-503	(6.5±1.2)(12)	0	1007±101	2
72 WAG/ZEL2 k_b .	EX	195-503	(5.8±1.2)(12)	0	1560±126	2
76 WHY/PAY $k_a + k_b$.	EX	215-460	(3.61±0.72)(13)	0	1233±50	2
77 MIC/LEE k_b . Discharge-flow. Resonance-fluorescence. $[H]_0 \sim 1.0 \times 10^{11}$ molec. cm^{-3} . $P(He) = 2$ torr.	EX	298	(3.79±0.24)(11)			2
$H + CH_2=C=CH_2 \rightarrow CH_3C=CH_2^\dagger$ (a) $\rightarrow CH_2CH=CH_2^\dagger$ (b) Hydrogen atom + 1,2-Propadiene (Allene)						
72 WAG/ZEL3 k_a .	EX	273-470	(8.5±2.0)(12)	0	1007±101	2
72 WAG/ZEL3 k_b .	EX	273-470	(4.0±2.0)(12)	0	1359±201	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
80 ALE/ARU1 ¹⁾ P = 4.0 torr.	EX	295	1.51(11)			2	
80 ALE/ARU1 ¹⁾ P = 3.9 torr.	EX	363	2.89(11)			2	
80 ALE/ARU1 ¹⁾ P = 4.0 torr.	EX	523	1.16(12)			2	
80 ALE/ARU1 ¹⁾ P = 4.9 torr.	EX	853	1.69(12)			2	
¹⁾ k _{overall} . Resonance-fluorescence. k values are given for other, lower pressures.							
H + CH ₃ CH=CH ₂ → H ₂ + CH ₂ =CHCH ₂ (a) → CH ₃ CH ₂ CH ₂ (b) → (CH ₃) ₂ CH (c) → CH ₃ + CH ₂ =CH ₂ (d)							
Hydrogen atom + 1-Propene							
72 FAL/SUN k _a /(k _b + k _c).	RL	298	2.0(-3)			2/2	
72 WAG/ZEL1 k _b .	EX	195-390	(4.4±0.6)(12)	0	1384±101	2	
78 MAR/PUR k _b /k _{ref} . 2,2,3,3-Tetramethylbutane pyrolysis. Static system. P = (3-19) torr. k _{ref} : H + (CH ₃) ₂ C=CH ₂ → (CH ₃) ₃ C Rate ratio determined on the basis of reaction: (CH ₃) ₃ CC(CH ₃) ₃ → (CH ₃) ₃ C + (CH ₃) ₃ C	RL	718	2.2			2/2	
71 COW/KEI ¹⁾ k _b + k _c . M = He. Discharge-flow. k increasing to (4.82±0.48)×10 ¹¹ cm ³ mol ⁻¹ s ⁻¹ for (0.96-4.91) torr.	EX	298	(4.00±0.36)(11)			2	
71 COW/KEI ¹⁾ (k _b + k _c)/k _{ref} . M = Ne, Ar. Steady-state photolysis method. P = (10-15) torr. k _{ref} : H + CH≡CH → CH ₂ =CH [†]	RL	298	(2.08±0.09)(1)			2/2	
71 COW/KEI ¹⁾ k _b + k _c . M = Ne, Ar. P = (10-15) torr. Steady-state photolysis method.	RN	298	(5.66±0.84)(11)			2	
¹⁾ The products of channels (b) and (c) are vibrationally excited.							
71 DAB/NIK k _b + k _c . M = He. P = (1.0-2.4) torr. The products of channels (b) and (c) are vibrationally excited.	EX	298	(4.55±0.26)(11)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref)), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
71 KUR/PET2 $k_b + k_c$. Resonance-fluorescence. The products of (b) and (c) are vibrationally excited. P(Total) = 50 torr.	EX	177-473	(6.13±0.16)(12)	0	609±6	2
75 MIH/SCH $k_b + k_c$. The products of channels (b) and (c) are vibrationally excited.	EX	295	(1.01±0.30)(12)			2
78 ISH/YAM $k_b + k_c$. Pulse-radiolysis. Resonance-absorption. Predominant paths. P(H ₂) = (200-1200) torr.	EX	298	(1.02±0.06)(12)			2
79 OKA/CVE ²) ($k_b + k_c$)/ k_{ref} . k_{ref} : H + NO + M → HNO + M	RL	298	(4.81±0.07)(-2)			2/3
79 OKA/CVE ²) $k_b + k_c$. ²) Modulated Hg-photosensitization. Chemiluminescence. The products are vibrationally excited. P = 50 torr.	RN	298	(8.33±0.16)(11)			2
82 HAR/PIT $k_b + k_c$. Flash-photolysis. Resonance-fluorescence. H atoms generated by pulsed vacuum-UV Photolysis of CH ₄ . Gas-chromatography. Predominant paths. The products of channels (b) and (c) are vibrationally excited. P(Total) = 50 torr.	EX	298-445	(1.33±0.15)(13)	0	785±54	2
82 WAT/KYO $k_b + k_c$. Pulse-radiolysis. Resonance-absorption. Gas-chromatography. P(H ₂) ~ 500 torr. P(CH ₃ CH=CH ₂) = (0.01-0.1) torr.	EX	200-500	(1.81±0.23)(13)	0	811±33	2
72 WAG/ZEL1 k_c .	EX	195-390	(5.4±0.6)(12)	0	629±50	2
74 LAU/BUE k_c/k_{ref} . k_{ref} : H + CH ₂ =CH ₂ → CH ₃ CH ₂ [†] . The products of channel (c) are vibrationally excited.	RL	298	(1.79±0.04)			2/2
75 CAM/MAR k_c . Determined from k_{-c} and published thermochemical data.	CO	676-813	6.31(12)	0	842	2
71 LEX/MAR1 k_d/k_c . M = Ar. Discharge flow method. The product of channel (c) is vibrationally excited. P(Ar) = (4-16) torr.	RL	290	(4.04±0.29)(-2)			2/2
72 KAL/KOR k_d .	EX	1073-1173	(4.52±0.90)(12)	0	0	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{H} + \text{CD}_3\text{CD}=\text{CD}_2 \rightarrow \text{CD}_3\text{CDHCD}_2$ (a) $\rightarrow \text{CD}_3\text{CDCD}_2\text{H}$ (b)							
Hydrogen atom + 1-Propene-1,1,2,3,3,3-d ₆							
82 WAT/KYO	EX	200-500	(1.54±0.34)(13)	0	759±64	2	
$k_a + k_b$. Pulse-radiolysis. Resonance-absorption. $P(\text{CD}_3\text{CD}=\text{CD}_2) = (0.01-0.1)$ torr. $P(\text{H}_2) \sim 500$ torr.							
$\text{D} + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CHDCH}_2$ (a) $\rightarrow \text{CH}_3\text{CHCH}_2\text{D}$ (b)							
Deuterium atom + 1-Propene							
71 DAB/NIK	EX	298	(6.20±0.66)(11)			2	
$k_a + k_b$. M = He. P = (0.6-2.2) torr. The products of channels (a) and (b) are vibrationally excited.							
75 MIH/SCH	EX	295	(6.87±0.24)(11)			2	
$k_a + k_b$. The products of channels (a) and (b) are vibrationally excited.							
79 ISH/SAT	EX	298	(7.83±1.20)(11)			2	
$k_a + k_b$. Pulse-radiolysis. Resonance-absorption.							
82 WAT/KYO	EX	200-500	(1.20±0.03)(13)	0	780±8	2	
$k_a + k_b$. Pulse-radiolysis. Resonance-absorption. $P(\text{CH}_3\text{CH}=\text{CH}_2) = (0.01-0.1)$ torr. $P(\text{D}_2) \sim 500$ torr.							
77 YAN	RL	1260-1360	(6.5±1.5)(-1)	0	0	2/2	
k_a/k_b . Estimated ratio. Thermolysis of 1-Propene in presence of D ₂ , in Ar, in a single shock-tube. $P(\text{D}_2) \sim 500$ torr.							
$\text{D} + \text{CD}_3\text{CD}=\text{CD}_2 \rightarrow \text{CD}_3\text{CD}_2\text{CD}_2$ (a) $\rightarrow (\text{CD}_3)_2\text{CD}$ (b)							
Deuterium atom + 1-Propene-1,1,2,3,3,3-d ₆							
82 WAT/KYO	EX	200-500	(1.33±0.16)(13)	0	799±34	2	
$k_a + k_b$. Pulse-radiolysis. Resonance-absorption. $P(\text{CD}_3\text{CD}=\text{CD}_2) = (0.01-0.1)$ torr. $P(\text{D}_2) \sim 500$ torr.							
$\text{H} + (\text{CH}_3)_2\text{CH} \rightarrow \text{H}_2 + \text{CH}_3\text{CH}=\text{CH}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_3$ (b)							
Hydrogen atom + Ethyl, 1-methyl-							
71 LEX/MAR1 ¹⁾	RL	290	(7.19±0.12)(-1)			2/2	
k_a/k_b . P(Ar) = (4-16) torr.							
71 LEX/MAR2 ¹⁾	RL	290	(5.4±1.1)(-1)			2/2	
k_a/k_b . P(Ar) = (4-12) torr.							
¹⁾ Discharge flow. The product of channel (b) is vibrationally excited.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref)), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
H + (CH₃)₂CH[†] → CH₃ + CH₃CH₂						
Hydrogen atom + Ethyl, 1-methyl-						
71 LEX/MAR1 Discharge-flow. P(Total) = (4-16) torr. (CH ₃)CH [†] assumed to be formed from H + CH ₃ CH=CH ₂ . k _{ref} : (CH ₃) ₂ CH [†] + M → (CH ₃) ₂ CH + M	RL	290	(4.84±0.28)(1)			2/2
H + CH₃CH₂CH₃ → H₂ + CH₃CH₂CH₂ (a)						
→ H ₂ + (CH ₃) ₂ CH (b)						
Hydrogen atom + Propane						
79 BAL/WAL1 k _a . A and B recalculated from an empirical formula proposed by the authors.	CO	753-773	1.32(14)	0	4715	2
76 SHE/KAL k _a + k _b .	EX	1123	3.7(12)			2
77 LED/VIL k _a + k _b .	EX	295	1.46(8)			2
78 LED/VIL k _a + k _b . Discharge-flow.	EX	281-1485	6.31(13)	0	3926±50	2 2.0
71 BAK/BAL k _b . Rate constant per secondary CH bond.	CO	298-753	5.1(13)	0	4253	2
79 BAL/WAL1 k _b . A and B recalculated from an empirical formula proposed by the authors.	CO	753-773	9.8(13)	0	4005	2
82 SHE/GUS k _b /k _a . Recalculated from the given secondary per primary bond rate constant ratio of 1.4±0.2. Pyrolysis of Propane/Isobutane mixtures, in a quartz flow-reactor. P = 100 torr.	RL	1023-1123	(4.7±0.7)(-1)			2/2
H + CH₂=CHCHO → products						
Hydrogen atom + 2-Propenal (Acrolein)						
78 KOD/NAK Fast flow-reactor. Time-of-flight Mass-spectrometry. P(Ar + H ₂) = 0.29 torr.	EX	298	(8.1±0.8)(11)			2
H + (CH₃)₂CO → H₂ + CH₃C(O)CH₂						
Hydrogen atom + 2-Propanone						
72 AZA/GYU	EX	843-928	(2.29±0.90)(14)	0	6995±755	2
76 AMB/BRA Discharge-flow. ESR detection.	EX	298-465	1.86(14)	0	3200±144	2 1.58

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$H + CH=CC=CH \rightarrow CH=CCH=CH^{\dagger}$ (a) $\rightarrow CH=CC=CH_2^{\dagger}$ (b)						
Hydrogen atom + 1,3-Butadiyne						
75 SCH/WAR $k_a + k_b$.	EX	298	1.3(12)			2
$H + CH_2=CHC=CH \rightarrow$ products						
Hydrogen atom + 1-Buten-3-yne						
75 SCH/WAR	ES	298	(2.0±0.2)(12)			2
$H + CH_2=CHCH=CH_2 (+M) \rightarrow CH_3CHCH=CH_2 (+M)$ (a) $\rightarrow CH_2CH_2CH=CH_2 (+M)$ (b) $\rightarrow H_2 + CH_2=CHCH=CH (+M)$ (c) $\rightarrow H_2 + CH_2=CHC=CH_2 (+M)$ (d)						
Hydrogen atom + 1,3-Butadiene						
71 DAB/NIK $k_a + k_b$. P(He) = 1.3 torr.	EX	298	(5.02±0.65)(12)			2
78 GOR/IVA2 ¹⁾	EX	305	(3.19±0.42)(11)			2
78 GOR/IVA2 ¹⁾ Lower-limit k.	EX	305	≥4.57(18)			3
¹⁾ $k_a + k_b$. Method based on collision-induced shifts and HF-transition line broadening in H atoms.						
79 ISH/SUG2 $k_a + k_b$. Pulse-radiolysis. Absorption-spectroscopy. P = (500-600) torr. H + (0.02-0.09) torr. O ₁ .	EX	298	(5.12±0.90)(12)			2
79 OKA/CVE ²⁾ ($k_a + k_b$)/ k_{ref} . k_{ref} : $H + NO + M \rightarrow HNO + M$.	RL	298	(2.76±0.05)(-1)			2/3
79 OKA/CVE ²⁾ $k_a + k_b$.	RN	298	(4.27±0.26)(12)			2
²⁾ Modulated Hg-photosensitization. Chemiluminescence. k might be slightly P-dependent. The products are vibrationally excited. P = 100 torr.						
75 NAM/SHE $k_a + k_b + k_c + k_d$.	EX	1073-1123	(1.6±0.3)(13)	0	0	2
$D + CH_2=CHCH=CH_2 \rightarrow CH_2DCHCH=CH_2$ (a) $\rightarrow CH_2CHDCH=CH_2$ (b)						
Deuterium atom + 1,3-Butadiene						
71 DAB/NIK $k_a + k_b$. M = He. P = (1.6-2.6) torr.	EX	298	(3.17±0.05)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 ISH/SUG2 $k_a + k_b$. Pulse-radiolysis. Absorption-spectroscopy. P = (500-600) torr. H_2 + (0.02-0.09) torr. OI.	EX	298	(4.52±0.36)(12)			2
$H + CH_3CH_2CH=CH_2 \rightarrow CH_3CH_2CHCH_3$ (a) $\rightarrow CH_3CH_2CH_2CH_2$ (b) $\rightarrow H_2 + CH_3CH_2CH=CH$ (c) $\rightarrow H + CH_3CH_2C=CH_2H$ (d) $\rightarrow H_2 + CH_3CHCH=CH_2$ (e) (or $H_2 + CH_3CH=CHCH_2$) $\rightarrow H_2 + CH_2CH_2CH=CH_2$ (f)						
Hydrogen atom + 1-Butene						
71 COW/KEI $k_a + k_b$. M = He. Discharge-flow. The products are vibrationally excited. P = 2.86 torr.	EX	298	(6.81±0.48)(11)			2
71 COW/KEI ¹⁾ ($k_a + k_b$)/ k_{ref} . k_{ref} : $H + CH=CH \rightarrow CH_2=CH^\dagger$	RL	298	(2.96±0.58)(1)			2/2
71 COW/KEI ¹⁾ $k_a + k_b$. ¹⁾ M = Na, Ar. Steady-state Photolysis. The products are vibrationally excited. P = (10-15) torr.	RN	298	(7.83±2.41)(11)			2
71 DAB/NIK $k_a + k_b$. M = Ha. P = (0.4-2.8) torr.	EX	298	(8.31±0.48)(11)			2
74 SHI/AMA ($k_a + k_b$)/($k_c + k_d + k_e + k_f$).	RL	923	1.5(1)			2/2
78 ISH/YAM $k_a + k_b$. Pulse-radiolysis. Resonance-absorption. Predominant paths. P(H_2) = (200-1200) torr.	EX	298	(1.20±0.30)(12)			2
79 OKA/CVE ²⁾ ($k_a + k_b$)/ k_{ref} . k_{ref} : $H + NO + M \rightarrow HNO + M$.	RL	298	(4.94±0.13)(-2)			2/3
79 OKA/CVE ²⁾ $k_a + k_b$. ²⁾ Hg-photosensitization. Chemiluminescence. The products are vibrationally excited. P = 50 torr.	RN	298	(8.36±0.16)(11)			2
82 HAR/PIT $k_a + k_b$. Flash-photolysis. Resonance-fluorescence. H atoms generated by pulsed vacuum-UV Photolysis of CH_4 . P(Total) = 50 torr.	EX	298-445	(2.27±0.24)(13)	0	942±94	2
74 SHI/AMA k_a/k_b .	RL	923	3.0			2/2
72 FAL/SUN $k_e/(k_a + k_b)$.	RL	298	1.6(-2)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$D + CH_3CH_2CH=CH_2 \rightarrow CH_3CH_2CHDCH_2$ (a) $\rightarrow CH_3CH_2CHCH_2D$ (b)						
Deuterium atom + 1-Butene						
71 DAB/NIK $k_a + k_b$. M = He. P = (0.6-2.6) torr.	EX	298	(8.25±0.60)(11)			2
79 ISH/SAT $k_a + k_b$. Pulse-radiolysis. Resonance-absorption.	EX	298	(9.64±0.60)(11)			2
$H + CH_3CH=CHCH_3 \rightarrow CH_3CHCH_2CH_3$ (a) $\rightarrow H_2 + CH_3CH=CHCH_2$ (b) $\rightarrow H_2 + CH_3CH=CCH_3$ (c)						
Hydrogen atom + 2-Butene (Unspecified form)						
74 SHI/AMA $k_a/(k_b + k_c)$.	RL	923	5.0			2/2
74 LAU/BUE k_a/k_{ref} . k_{ref} : $H + CH_2=CH_2 \rightarrow CH_3CH_2^\dagger$ The product is vibrationally excited.	RL	298	(8.3±0.13)(-1)			2/2
$H + cis-CH_3CH=CHCH_3 \rightarrow H_2 + CH_3CH=CHCH_2$ (a) $\rightarrow H_2 + CH_3CHCH=CH_2$ (b) $\rightarrow CH_3CH_2CH(\cdot)CH_3$ (c)						
Hydrogen atom + 2-Butene, (Z)-						
72 FAL/SUN $(k_a + k_b)/k_c$.	RL	298	1.5(-2)			2/2
71 COW/KEI k_c . M = He. P = 3.24 torr. Discharge-flow. The product is vibrationally excited.	EX	298	(3.85±0.30)(11)			2
71 COW/KEI ¹⁾ k_c/k_{ref} . k_{ref} : $H + CH\equiv CH \rightarrow CH_2=CH^\dagger$	RL	298	(9.1±0.9)			2/2
71 COW/KEI ¹⁾ k_c .	RN	298	(2.47±0.60)(11)			2
¹⁾ M = He. P = (10-15) torr. Steady-state Photolysis. The product is vibrationally excited.						
71 DAB/NIK k_c . M = He. P = (1.1-2.8) torr.	EX	298	(4.75±0.35)(11)			2
78 ISH/YAM k_c . Pulse-radiolysis. Resonance-absorption. The product is vibrationally excited. Predominant path. $P(H_2) = (200-1200)$ torr.	EX	298	(6.02±0.60)(11)			2
79 OKA/CVE ²⁾ k_{ref} : $H + NO + M \rightarrow HNO + M$.	RL	298	(2.29±0.05)(-2)			2/3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
79 OKA/CVE ²⁾ ²⁾ k _c . Hg-photosensitization. Chemiluminescence. The product is vibrationally excited. P = 50 torr.	RN	298	(3.62±0.06)(11)			2	
82 HAR/PIT k _c . Flash-photolysis. Resonance-fluorescence. H atoms generated by pulsed vacuum-UV Photolysis of CH ₄ . Gas-chromatography. P(Total) = 50 torr.	EX	298-445	(1.74±0.18)(13)	0	1083±86	2	
D + cis-CH ₃ CH=CHCH ₃ → CH ₃ CHDCHCH ₃ Deuterium atom + 2-Butene, (Z)-							
71 DAB/NIK M = He. P = (0.6-2.6) torr.	EX	298	(4.07±0.22)(11)			2	
79 ISH/SAT Pulse-radiolysis. Resonance-absorption.	EX	298	(4.82±0.60)(11)			2	
H + trans-CH ₃ CH=CHCH ₃ → H ₂ + CH ₃ CH=CHCH ₂ (a) → H ₂ + CH ₃ CHCH=CH ₂ (b) → CH ₃ CH ₂ CHCH ₃ (c) Hydrogen atom + 2-Butene, (E)-							
72 FAL/SUN (k _a + k _b)/k _c .	RL	298	9.0(-3)			2/2	
71 COW/KEI k _c . M = He. Discharge-flow. The product is vibrationally excited. P = 1.79 torr.	EX	298	(4.28±0.24)(11)			2	
71 COW/KEI ¹⁾ k _c /k _{ref} . k _{ref} : H + CH=CH → CH ₂ =CH [†]	RL	298	(1.19±0.14)(1)			2/2	
71 COW/KEI ¹⁾ k _c . ¹⁾ M = Ne, Ar. P = (10-15) torr. Steady-state Photolysis. The product is vibrationally excited.	RN	298	(3.25±0.84)(11)			2	
71 DAB/NIK k _c . M = He. P = (0.4-1.9) torr.	EX	298	(5.38±0.41)(11)			2	
78 ISH/YAM k _c . Pulse-radiolysis. Resonance-absorption. Predominant path. P(H ₂) = (200-1200) T	EX	298	(6.63±1.20)(11)			2	
78 KOD/NAK k _c . Fast-flow. P(Ar + H ₂) = 0.20 torr.	EX	298	(5.1±0.5)(11)			2	
79 OKA/CVE ²⁾ k _{ref} : H + NO + M → HNO + M.	RL	298	(2.65±0.05)(-2)			2/3	
79 OKA/CVE ²⁾ ²⁾ k _c . Hg-photosensitization. Chemiluminescence. The product is vibrationally excited. P = 50 torr.	RN	298	(4.55±0.08)(11)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 HAR/PIT k_c . Resonance-fluorescence. H atoms generated by photolysis of CH_4 . P(Total) = 50 torr.	EX	298-445	(2.08±0.21)(13)	0	1043±63	2	
D + trans- $\text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CHDCHCH}_3$							
Deuterium atom + 2-Butene, (E)-							
71 DAB/NIK M = He. P = (0.7-2.2) torr.	EX	298	(4.66±0.14)(11)			2	
79 ISH/SAT Pulse-radiolysis. Resonance-absorption. Predominant path.	EX	298	(4.82±0.60)(11)			2	
H + $(\text{CH}_3)_2\text{C}=\text{CH}_2$ (+ M) $\rightarrow$ $(\text{CH}_3)_3\text{C}$ (+ M) (a)							
$\rightarrow (\text{CH}_3)_2\text{CHCH}_2$ (+ M) (b)							
$\rightarrow \text{H}_2 + \text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ (+ M) (c)							
$\rightarrow \text{CH}_3 + \text{CH}_3\text{CH}=\text{CH}_2$ (+ M) (d)							
Hydrogen atom + 1-Propene, 2-methyl-							
76 BRA/WES1 k_a . Computer-fit to a proposed mechanism.	DE	1030-1300	1.6(13)	0	758	2	1.95
81 CAN/MAR1 k_a . Discharge-flow system. Mass-Spectrometry. P(Total) = (7-8) torr.	EX	298-563	3.89(13)	0	901±96	2	1.29
78 GOR/IVA2 $k_a + k_b$. Collision-induced shifts and HF-transition line broadening in H-atoms.	EX	305	(2.18±0.04)(12)			2	
78 GOR/IVA2 $k_a + k_b$. H-maser relaxation method.	EX	305	(2.17±0.60)(12)			2	
78 GOR/IVA2 $k_a + k_b$. Collision-induced shifts. HF-transition line broadening in H-atoms. Lower-limit k.	EX	305	≥3.08(18)			3	
78 HOR/CAL ($k_a + k_b$)/ k_{ref} . HCHO Photolysis at 313 nm. P(HCHO) = (1-12) torr. k_{ref} : $\text{H} + \text{HCHO} \rightarrow \text{H}_2 + \text{CHO}$.	RL	298	(4.3±0.4)(1)			2/2	
78 ISH/YAM $k_a + k_b$. Pulse-radiolysis. Resonance-absorption. Predominant paths. P(H_2) = (200-1200) torr.	EX	298	(3.13±0.36)(12)			2	
79 OKA/CVE ¹⁾ ($k_a + k_b$)/ k_{ref} . k_{ref} : $\text{H} + \text{NO} + \text{M} \rightarrow \text{HNO} + \text{M}$.	RL	298	(1.56±0.04)(-1)			2/3	
79 OKA/CVE ¹⁾ $k_a + k_b$.	RN	298	(2.43±0.09)(12)			2	
¹⁾ Hg-photosensitization. Chemiluminescence. The products vibrationally excited. P = 50 torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 HAR/PIT k _a + k _b . Flash-photolysis. Resonance-fluorescence. Gas-chromatography. H atoms generated by photolysis of CH ₄ . P(Total) = 50 torr.	EX	298-445	(3.68±0.36)(13)	0	849±98	2
71 COW/KEI ²⁾ (k _a + k _d)/k _{ref} . k _{ref} : H + CH≡CH → CH ₂ =CH [†]	RL	298	(7.45±1.49)(1)			2/2 1.48
71 COW/KEI ²⁾ k _a + k _d .	RL	298	(2.05±0.60)(12)			2
²⁾ M = Ne, Ar. P = (10-15) torr. Steady-state Photolysis. Products vibrationally excited.						
76 BRA/WES2 k _b /k _a . Computer-fit to a proposed mechanism.	RL	1055-1325	6.76(-2)	0	-2382	2/2 1.48
78 MAR/PUR k _b /k _c . 2,2,3,3-Tetramethylbutane pyrolysis in a static system. P = (3-19) torr. Rate-ratio determined on the basis of reaction: (CH ₃) ₃ CC(CH ₃) ₃ → (CH ₃) ₃ C + (CH ₃) ₃ C	RL	718	9.4(-1)			2/2
71 LEX/MAR2 k _d /k _a . M = Ar. Discharge flow. P(Ar) = (4-12) torr.	RL	290	(1.4±0.3)(-3)			2/2
80 MAR/CAN k _d /k _a . M = Ar. Discharge-flow. Products of (a) vibrationally excited. P(Ar) = 6.6 torr.	RL	293-601	2.95	0	1997±313	2/2
D + (CH ₃) ₂ C=CH ₂ → (CH ₃) ₂ CDCH ₂ (a) → (CH ₃) ₂ CCH ₂ D (b)						
Deuterium + 1-Propene, 2-methyl-						
71 DAB/NIK M = He. P = (1.0-2.2) torr.	EX	298	(2.02±0.09)(12)			2
79 ISH/SAT k _a + k _b . Pulse-radiolysis. Resonance-absorption.	EX	298	(2.29±0.18)(12)			2
H + (CH ₃) ₃ C → (CH ₃) ₃ CH (a) → H ₂ + (CH ₃) ₂ C=CH ₂ (b)						
Hydrogen atom + Ethyl, 1,1-dimethyl-						
71 LEX/MAR2 k _b /k _a . M = Ar. Discharge flow. Product of step (a) vibrationally excited. P(Ar) = (4-12) torr.	RL	290	(3.73±0.12)			2/2
80 MAR/CAN k _b /k _a . M = Ar. Discharge-flow. P(Ar) = 6.6 torr. T-independent ratio.	RL	293-601	(3.55±0.24)	0	0	2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{H} + (\text{CH}_3)_3\text{C}^\dagger \rightarrow \text{CH}_3 + (\text{CH}_3)_2\text{CH} \quad (\text{a})$ $\rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2 \quad (\text{b})$						
Hydrogen atom + Ethyl, 1,1-dimethyl-						
71 LEX/MAR2 ¹⁾ k_a/k_{ref}	RL	290	(4.58±1.0)			2/2
71 LEX/MAR2 ¹⁾ k_b/k_{ref}	RL	290	(7.68±0.54)(-1)			2/2
¹⁾ M = Ar. Discharge flow. P(Ar) = (4-12) torr. $k_{\text{ref}}: (\text{CH}_3)_3\text{C}^\dagger + \text{M} \rightarrow (\text{CH}_3)_3\text{C} + \text{M}$						
$\text{H} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 \quad (\text{a})$ $\rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CHCH}_3 \quad (\text{b})$						
Hydrogen atom + Butane						
79 BAL/WAL1 k_a . A and B recalculated by an empirical formula.	CO	753-773	1.32(14)	0	4715	2
76 YAM/NAM $k_a + k_b$.	EX	980-1050	(9.64±2.53)(11)	0	0	2
71 BAK/BAL k_b . Rate constant per secondary CH bond.	CO	298-753	5.5(13)	0	4253	2
79 BAL/WAL1 k_b . A and B recalculated by an empirical formula.	CO	753-773	1.96(14)	0	4005	2
$\text{H} + (\text{CH}_3)_3\text{CH} \rightarrow \text{H}_2 + (\text{CH}_3)_3\text{C} \quad (\text{a})$ $\rightarrow \text{H}_2 + (\text{CH}_3)_2\text{CHCH}_2 \quad (\text{b})$						
Hydrogen atom + Propane, 2-methyl-						
71 BAK/BAL k_a . Rate constant per tertiary CH bond.	CO	298-753	8.7(13)	0	3553	2
79 BAL/WAL1 ¹⁾ k_a .	CO	753-773	5.1(13)	0	3030	2
79 BAL/WAL1 ¹⁾ k_b .	CO	753-773	1.99(14)	0	4715	2
¹⁾ A and B recalculated by an empirical formula.						
82 SHE/GUS ²⁾ $(k_a + k_b)/k_{\text{ref}}$ $k_{\text{ref}}: \text{H} + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{H}_2 + (\text{CH}_3)_2\text{CH} \quad (\text{c})$ $\rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}_2 \quad (\text{d})$	RL	1023-1123	(2.2±0.2)	0	0	2/2
82 SHE/GUS ²⁾ k_a/k_b . Recalculated from the reported tertiary per primary bond rate constant ratio of 10.5	RL	1023-1123	1.17	0	0	2/2
²⁾ Pyrolysis of Propane/Isobutane mixtures, in a quartz flow-reactor. P = 100 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 SHE/IVA $k_a + k_b$. Pyrolysis of $(CH_3)_3CH$ in various flow-reactors. P = (100-750) torr.	EX	1023-1073	$(8.0 \pm 0.9)(12)$	0	0	2
$H + (CH_3)_3COH \rightarrow H_2O + (CH_3)_3C$ Hydrogen atom + 2-Propanol, 2-methyl-						
73 ADE	EX	520-770	4.0(13)	0	4126	2
73 ADE/WAG2	EX	295-700	$(4.0 \pm 0.4)(13)$	0	4127 ± 302	2
$H + (CH_3CH_2)_2O \rightarrow H_2 + CH_3CH_2OCHCH_3$ Hydrogen atom + Ethane, 1,1'-oxybis- (Diethyl ether)						
79 FAU/HOY Isothermal discharge-flow. Mass-spectrometry. Electron-Spin-Resonance. Gas-chromatography.	EX	250-620	$(7.4 \pm 3.6)(12)$	0	1630 ± 100	2
$H + $  $\rightarrow CH_2CH_2CH_2CH_2SH$ Hydrogen atom + Thiophene, tetrahydro-						
78 HOR/NIS Discharge-flow technique. P ~ 5 torr.	DE	295-576	8.5(12)	0	1010	2
$H + CH_3CH_2CH_2CH_2SH \rightarrow H_2 + CH_3CH_2CH_2CH_2S$ (a) $\rightarrow H_2S + CH_3CH_2CH_2CH_2$ (b) Hydrogen atom + 1-Butanethiol						
78 HOR/NIS ¹⁾ k_a .	DE	295-576	1.3(13)	0	1600	2
78 HOR/NIS ¹⁾ k_b .	DE	295-576	1.6(12)	0	1119	2
¹⁾ Discharge-flow technique. P ~ 5 torr.						
$H + (CH_3CH_2)_2S \rightarrow CH_3CH_2SH + CH_3CH_2$ Hydrogen atom + Ethane, 1,1'-thiobis-						
81 EKW/SAF2 H atoms generated by Hg-photosensitized decomposition of H_2 . General-vacuum apparatus. Gas-chromatography. k determined relative to the reaction: $H + CH_2=CH_2 \rightarrow CH_3CH_2$. P(H_2) ~ 580 torr. P(Diethylsulfide) = (1-32) torr.	RN	298-461	$(4.7 \pm 0.9)(13)$	0	1911 ± 77	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{H} + \text{CH}_3\text{CH}_2\text{SSCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{SH} + \text{CH}_3\text{CH}_2\text{S}$ Hydrogen atom + Disulfide, diethyl-						
81 EKW/SAF1 H atoms generated by Hg-photosensitized decomposition of H_2 . General-vacuum apparatus. Gas-chromatography. P(Diethyldisulfide) = (2-15) torr. P(H_2) ~ 580 torr.	EX	298-418	(4.73±0.64)(13)	0	861±35	2
$\text{H} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ (b) $\rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CHCH}=\text{CH}_2$ (c) $\rightarrow \text{H}_2 + \text{CH}_3\text{CHCH}_2\text{CH}=\text{CH}_2$ (d) $\rightarrow \text{H}_2 + \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ (e) Hydrogen atom + 1-Pentene						
71 COW/KEI $k_a + k_b$. M = He. Discharge-flow. The products are vibrationally excited. P = 3 torr.	EX	298	(6.38±0.48)(11)			2
71 COW/KEI ¹⁾ ($k_a + k_b$)/ k_{ref} . k_{ref} : $\text{H} + \text{CH}=\text{CH} \rightarrow \text{CH}_2=\text{CH}^\dagger$	RL	298	(2.86±0.48)(1)			2/2
71 COW/KEI ¹⁾ $k_a + k_b$. ¹⁾ M = Ne, Ar. Steady-state Photolysis. The products are vibrationally excited. P = (10-15) torr.	RN	298	(7.78±2.41)(11)			2
74 SHI/AMA ($k_a + k_b$)/($k_c + k_d + k_e$).	RL	923	9.0			2/2
74 SHI/AMA k_a/k_b .	RL	923	3.0			2/2
$\text{H} + \text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CHCH}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CHCH}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3$ (b) $\rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_2$ (c) $\rightarrow \text{H}_2 + \text{CH}_3\text{CHCH}=\text{CHCH}_3$ (d) $\rightarrow \text{H}_2 + \text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3$ (e) Hydrogen atom + 2-Pentene (Unspecified form)						
74 SHI/AMA k_a/k_b .	RL	923	1.0			2/2
74 SHI/AMA ($k_a + k_b$)/($k_c + k_d + k_e$).	RL	923	3.0			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{H} + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2$ (b) $\rightarrow \text{H}_2 + \text{CH}_3\text{CHC}(\text{CH}_3)=\text{CH}_2$ (c) $\rightarrow \text{H}_2 + \text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ (d) $\rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{C}(=\text{CH}_2)\text{CH}_2$ (e)						
Hydrogen atom + 1-Butene, 2-methyl-						
71 DAB/NIK $k_a + k_b$. M = He. P = (0.7-1.3) torr.	EX	298	(9.09±0.96)(11)			2
74 SHI/AMA k_a/k_b .	RL	923	4.0			2/2
74 SHI/AMA $(k_a + k_b)/(k_c + k_d + k_e)$.	RL	923	1.3(1)			2/2
$\text{D} + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)\text{CH}_2\text{D}$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CD}(\text{CH}_3)\text{CH}_2$ (b)						
Deuterium atom + 1-Butene, 2-methyl-						
71 DAB/NIK $k_a + k_b$. M = He. P = (1.2-2.6) torr.	EX	298	(2.05±0.10)(12)			2
$\text{H} + (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCHCH}_3$ (a) $\rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2$ (b)						
Hydrogen atom + 1-Butene, 3-methyl-						
71 DAB/NIK $k_a + k_b$. M = He. P = (0.6-2.7) torr.	EX	298	(7.35±0.60)(11)			2
$\text{D} + (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCHCH}_2\text{D}$ (a) $\rightarrow (\text{CH}_3)_2\text{CHCHDCH}_2$ (b)						
Deuterium atom + 1-Butene, 3-methyl-						
71 DAB/NIK $k_a + k_b$. M = He. P = (0.6-2.6) torr.	EX	298	(7.65±0.60)(11)			2
$\text{H} + \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2$ (a) $\rightarrow \text{CH}_3\text{CHCH}(\text{CH}_3)_2$ (b) $\rightarrow \text{H}_2 + \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)\text{CH}_2$ (c) $\rightarrow \text{H}_2 + \text{CH}_2\text{CH}=\text{C}(\text{CH}_3)_2$ (d)						
Hydrogen atom + 2-Butene, 2-methyl- (Trimethylethylene)						
71 DAB/NIK $k_a + k_b$. M = He. P = (0.7-1.3) torr.	EX	298	(8.19±1.02)(11)			2
74 LAU/BUE $(k_a + k_b)/k_{\text{ref}}$. $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2^\dagger$ The products are vibrationally excited.	RL	298	(1.25±0.29)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
74 SHI/AMA k_a/k_b .	RL	923	4.0			2/2
74 SHI/AMA $(k_a + k_b)/(k_c + k_d)$.	RL	923	3.0			2/2
78 ISH/YAM $k_a + k_b$. Pulse-radiolysis. Resonance-absorption.	EX	298	(1.45±0.18)(12)			2
D + CH ₃ CH=C(CH ₃) ₂ → CH ₃ CHCD(CH ₃) ₂ (a) → CH ₃ CHDC(CH ₃) ₂ (b)						
Deuterium atom + 2-Butene, 2-methyl-						
71 DAB/NIK $k_a + k_b$. M = He. P = (0.6-2.6) torr.	EX	298	(9.22±0.54)(11)			2
79 ISH/SAT $k_a + k_b$. Pulse-radiolysis. Resonance-absorption.	EX	298	(1.20±0.18)(12)			2
H + CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ → H ₂ + CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ (a) → H ₂ + CH ₃ CH ₂ CH ₂ CHCH ₃ (b) → H ₂ + CH ₃ CH ₂ CHCH ₂ CH ₃ (c)						
Hydrogen atom + Pentane						
79 BAL/WAL1 ¹⁾ k_a .	CO	753-773	1.32(14)	0	4715	2
79 BAL/WAL1 ¹⁾ $k_b + k_c$.	CO	753-773	2.94(14)	0	4005	2
¹⁾ A and B recalculated by an empirical formula.						
H + (CH ₃) ₂ CHCH ₂ CH ₃ → H ₂ + CH ₂ CH(CH ₃)CH ₂ CH ₃ (a) → H ₂ + (CH ₃) ₂ CHCH ₂ CH ₂ (b) → H ₂ + (CH ₃) ₂ CHCHCH ₃ (c) → H ₂ + (CH ₃) ₂ CCH ₂ CH ₃ (d)						
Hydrogen atom + Butane, 2-methyl-						
79 BAL/WAL1 ¹⁾ $k_a + k_b$.	CO	753-773	1.98(14)	0	4715	2
79 BAL/WAL1 ¹⁾ k_c .	CO	753-773	9.8(13)	0	4005	2
79 BAL/WAL1 ¹⁾ k_d .	CO	753-773	5.1(13)	0	3030	2
¹⁾ A and B recalculated by an empirical formula.						
H + (CH ₃) ₄ C → H ₂ + (CH ₃) ₃ CCH ₂						
Hydrogen atom + Propane, 2,2-dimethyl- (Neopentane)						
76 BAK/BAL k_{ref} : O ₂ + H → O + OH. Optimization.	RL	753	5.2(1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 BAK/BAL	ES	753	2.4(11)			2
79 BAL/WAL1	CO	753-773	2.64(14)	0	4715	2
A and B recalculated by an empirical formula.						
H + (CH₃)₃COCH₃ → products						
Hydrogen atom + Propane, 2-methoxy-2-methyl-						
79 FAU/HOY	EX	250-620	(1.4±0.8)(14)	0	3750±150	2
Isothermal discharge-flow.						
Electron-Spin-Resonance.						
Gas-chromatography.						
Mass-spectrometry.						
H + CH₃CH₂CH₂C(CH₃)=CH₂ → CH₃CH₂CH₂C(CH₃)₂ (a)						
→ CH ₃ CH ₂ CH ₂ CH(CH ₃)CH ₂ (b)						
→ H ₂ + CH ₃ CH ₂ CHC(CH ₃)=CH ₂ (c)						
→ H ₂ + CH ₂ CH ₂ CH ₂ C(CH ₃)=CH ₂ (d)						
→ H ₂ + CH ₃ CH ₂ CH ₂ C(=CH ₂)CH ₂ (e)						
Hydrogen atom + 1-Pentene, 2-methyl-						
74 SHI/AMA	RL	923	4.0			2/2
k _a /k _b .						
74 SHI/AMA	RL	923	8.0			2/2
(k _a + k _b)/(k _c + k _d + k _e).						
H + CH₃CH₂CH=C(CH₃)₂ → CH₃CH₂CH₂C(CH₃)₂ (a)						
→ CH ₃ CH ₂ CHCH(CH ₃) ₂ (b)						
→ H ₂ + CH ₃ CH ₂ CH=C(CH ₃)CH ₂ (c)						
→ H ₂ + CH ₃ CHCH=C(CH ₃) ₂ (d)						
Hydrogen atom + 2-Pentene, 2-methyl-						
74 SHI/AMA	RL	923	3.0			2/2
k _a /k _b .						
74 SHI/AMA	RL	923	3.0			2/2
(k _a + k _b)/(k _c + k _d).						
H + CH₃CH₂C(CH₃)=CHCH₃ → CH₃CH₂C(CH₃)CH₂CH₃ (a)						
→ CH ₃ CH ₂ CH(CH ₃)CHCH ₃ (b)						
→ H ₂ + CH ₃ CH ₂ C(CH ₃)=CHCH ₂ (c)						
→ H ₂ + CH ₃ CHC(CH ₃)=CHCH ₃ (d)						
→ H ₂ + CH ₃ CH ₂ C(=CH ₂)CH ₃ (e)						
Hydrogen atom + 2-Pentene, 3-methyl-						
74 SHI/AMA	RL	923	3.0			2/2
k _a /k _b .						
74 SHI/AMA	RL	923	3.0			2/2
(k _a + k _b)/(k _c + k _d + k _e).						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{H} + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CCH}(\text{CH}_3)_2$ Hydrogen atom + 2-Butene, 2,3-dimethyl- (Tetramethylethylene)						
71 DAB/NIK M = He. P = (0.7-1.3) torr.	EX	298	(6.99±0.30)(1)			2
$\text{D} + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CCD}(\text{CH}_3)_2$ Deuterium atom + 2-Butene, 2,3-dimethyl- (Tetramethylethylene)						
71 DAB/NIK M = He. P = (0.6-2.6) torr.	EX	298	(8.55±0.78)(11)			2
$\text{D} + \text{C}_6\text{H}_{12} \rightarrow \text{DH} + \text{C}_6\text{H}_{11}^\bullet$ Deuterium atom + Cyclohexane → Deuterium hydride + Cyclohexyl						
75 KIM/TIM Reaction of D atom with Cyclohexane in an ESR-flow. Mass-spectrometry. [Cyclohexane] = (0.48-1.32)10 ¹⁴ molec.cm ⁻³ . P = (0.33-0.94) torr.	EX	297-596	(4.1±1.0)(13)	0	2013±151	2
$\text{H} + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}_2$ (a) $\rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CHCH}_3$ (b) $\rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_2\text{CH}_3$ (c) $\rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CHCH}_2\text{CH}_2\text{CH}_3$ (d)						
Hydrogen atom + Hexane						
81 SHE/RUM ¹⁾	EX	973	(8.8±2.7)(12)			2
81 SHE/RUM ¹⁾	EX	1028	(8.7±2.2)(12)			2
¹⁾ k _a + k _b + k _c + k _d . Flow-reactor with powdered-quartz-fluidized bed. P(Hexane) = (10-50) torr. P(Total) = 100 torr.						
$\text{H} + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{H}_2 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}_2$ (a) $\rightarrow \text{H}_2 + (\text{CH}_3)_2\text{CCH}(\text{CH}_3)_2$ (b)						
Hydrogen atom + Butane, 2,2-dimethyl-						
75 BUL/MAR k _b /k _a . Estimated ratio. Static System pyrolysis.	RL	667-770	1.0(-1)	0	-2526	2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{H} + (\text{CH}_3)_2\text{CHN}=\text{NCH}(\text{CH}_3)_2$ $\rightarrow \text{H}_2 + \text{CH}_2\text{CH}(\text{CH}_3)\text{N}=\text{NCH}(\text{CH}_3)_2$ (a) $\rightarrow (\text{CH}_3)_2\text{CHNHNCH}(\text{CH}_3)_2$ (b)						
Hydrogen atom + Diazene, bis(1-methylethyl)- (Azoisopropane)						
72 ARI/STE k_a/k_b . Azoisopropane Photolysis.	RL	295	(1.0±0.15)(-1)			2/2
$\text{H} + (\text{CH}_3)_3\text{CCH}(\text{CH}_3)_2 \rightarrow \text{H}_2 + (\text{CH}_3)_3\text{CC}(\text{CH}_3)_2$ (a) $\rightarrow \text{H}_2 + \text{CH}_2(\text{CH}_3)_2\text{CCH}(\text{CH}_3)_2$ (b) $\rightarrow \text{H}_2 + (\text{CH}_3)_3\text{CCH}(\text{CH}_3)\text{CH}_2$ (c)						
Hydrogen atom + Butane, 2,2,3-trimethyl-						
81 BAL/WAL2 ¹⁾ k_a/k_{ref} . $k_{\text{ref}}: \text{H} + \text{O}_2 \rightarrow \text{OH} + \text{O}$. Estimated ratio.	RL	753	1.64(2)			2/2
81 BAL/WAL2 ¹⁾ $(k_b + k_c)/k_{\text{ref}}$. $k_{\text{ref}}: \text{H} + \text{O}_2 \rightarrow \text{OH} + \text{O}$. Estimated ratio.	RL	753	9.3(1)			2/2
81 BAL/WAL2 ¹⁾ $(k_a + k_b + k_c)/k_{\text{ref}}$. $k_{\text{ref}}: \text{H} + \text{O}_2 \rightarrow \text{OH} + \text{O}$. Optimization.	RL	753	2.57(2)			2/2
81 BAL/WAL2 ¹⁾ $k_a + k_b + k_c$.	SE	753	1.48(12)			2
¹⁾ Oxidation of 2,2,3-Trimethylbutane in H_2/O_2 mixtures, in aged boric acid- coated reaction vessels. Gas-chromatography. P(2,2,3-Trimethylbutane) = 5 torr. P(Total) = 500 torr.						
$\text{H} + (\text{CH}_3)_3\text{CC}(\text{CH}_3)_3 \rightarrow \text{H}_2 + (\text{CH}_3)_3\text{CC}[(\text{CH}_3)_2]\text{CH}_2$ Hydrogen atom + Butane, 2,2,3,3-tetramethyl						
78 MAR/PUR 2,2,3,3-Tetramethylbutane pyrolysis in a static system. P = (3-19) torr. k_{ref} : $\text{H} + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow \text{H}_2 + \text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ Rate ratio determined on the basis of reaction: $(\text{CH}_3)_3\text{CC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_3\text{C} + (\text{CH}_3)_3\text{C}$	RL	699-735	1.0(1)	0	2045±3609	2/2 100.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
H₂ (+ M) → H + H (+ M)							
Hydrogen molecule							
73 BRE/BIR M = H.	EX	3500-8000	2.12(15)	0	43885	2	
73 BRE/BIR M = H ₂ .	EX	3500-8000	3.30(15)	0	52944	2	
73 BRE/BIR M = Ar.	EX	3500-8000	9.35(13)	0	44741	2	
73 BRE/BIR M = Xe.	EX	3500-8000	9.35(13)	0	44741	2	
D₂ (+ M) → D + D (+ M)							
Deuterium molecule							
75 APP/APP	EX	1800-4000	1.45(14)	0	47006	2	
H₂ + D₂ → HD + HD							
Hydrogen molecule + Deuterium molecule							
77 LIF/FRE	ES	1200-1516	1.26(14)	0	19124±2516	2	6.31
HD + HD → H₂ + D₂							
Deuterium hydride							
72 NIK/MAI Pressure-normalized rate constant.	EX	833-1022	1.26(22)	0	28083±1808	2	15.85
H₂ + NO → H + HNO							
Hydrogen molecule + Nitrogen oxide (NO)							
75 KOS/AND	EX	2000-4000	3.98(13)	0	29039	2	
76 AND/ASA Reevaluation of the experimental data reported in 75 KOS/AND by using a computer simulation method.	DE	2300-3500	3.16(13)	0	27781	2	1.41

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units factor	k err. factor
H₂(v>5) + NO → H + HNO							
Hydrogen molecule + Nitrogen oxide (NO)							
80 DOD/ZEL High-frequency discharge. Mass-spectrometry.	EX	295	(1.20±0.60)(13)				2
H₂ + NO₂ → H + HONO							
Hydrogen molecule + Nitrogen oxide (NO ₂)							
78 SLA/GRI2 Shock-waves. Fit to experimental data. P = (1-4) atm.	ES	760-1000	(2.4±1.0)(13)	0	14595±503		2
H₂ + N₂O → H₂O + N₂							
Hydrogen molecule + Nitrogen oxide (N ₂ O)							
78 ROO/HAN Shock-waves. Estimated k on the basis of a suggested mechanism. The preexponential factor expressed as: A(T/298) ^{0.5} .	ES	1700-3000	3.45(12)	0.5	0		2
H₂(X¹Σ_g⁺) + C₂(X¹Σ_g⁺) → H(2S) + CH≡C(X²Σ⁺) (a) → CH≡CH (b)							
Hydrogen molecule + Carbon dimer							
79 PAS/MCD k _a . Multiphoton laser photodissociation of CF ₃ C≡CCF ₃ . Laser-induced fluorescence.	EX	298	(8.31±0.36)(11)				2
82 PIT/PAS k _b . Dye-laser induced fluorescence. Carbon dimers produced by multiphoton UV-photolysis of CF ₃ C≡CCF ₃ .	EX	300-600	(1.07±0.66)(14)	0	1470±216		2
80 REI/MAN2 k _{overall} . IR Multiple photon dissociation CH ₂ =CHCN or CHCl=CCl ₂ . Laser-induced Fluorescence.	EX	300	(8.43±1.20)(11)				2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/(ref), A,A/(ref)	n	B, B-B(ref)	k,A units	k err. factor
$H_2(X^1\Sigma_g^+) + C_2(a^3\Pi_u) \rightarrow H(^2S) + CH\equiv C(X^2\Sigma^+) \text{ (a)}$ → any other products (b)							
Hydrogen molecule + Carbon dimer							
81 PAS/PIT k_a . Multiple photon laser dissociation of $CF_3C\equiv CCF_3$ or C_6H_6 . Laser-Induced Fluorescence.	EX	300-600	(9.34±0.60)(12)	0	3012±31	2	
80 REI/MAN2 $k_a + k_b$. IR Multiple photon dissociation of of $CH_2=CHCN$ or $CHCl=CCl_2$. Laser-induced Fluorescence. Upper-limit k.	EX	300	<1.81(10)			2	
$D_2 + C_2(a^3\Pi_u) \rightarrow D + CD\equiv C$							
Deuterium molecule + Carbon dimer							
81 PAS/PIT Multiple photon laser dissociation of $CF_3C\equiv CCF_3$ or C_6H_6 . Laser-induced Fluorescence.	EX	300-600	(1.08±0.13)(13)	0	3710±72	2	
$H_2 + C_2O \rightarrow \text{products}$							
Hydrogen molecule + Carbon oxide (C_2O)							
80 DON/PIT Laser photodissociation of C_3O_2 at 266 nm. Dye-laser Induced Fluorescence. Upper-limit k.	EX	298	<1.20(11)			2	
$D_2 + CH\equiv CH \rightarrow CHD=CHD$							
Deuterium molecule + Ethyne							
77 OGU2	EX	1000-1600	(4.9±1.3)(11)	0	17564±302	2	
$H_2 + C_3 \rightarrow \text{products}$							
Hydrogen molecule + Carbon trimer							
80 REI/MAN1 IR Multiphoton dissociation of Allene. Time-Resolved Chemiluminescence. Upper-limit k.	EX	300	≤1.80(10)			2	
$H_2 + \text{Cyclohexadiene} \rightarrow \text{Cyclohexene}$							
72 DEM/HUY Pyrolysis in a cylindrical Pyrex reaction vessel. Gas-chromatography. Mass-spectrometry. P = (10-500) torr.	EX	512-673	1.78(13)	0	18319±554	2	2.51

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + O₃ → HO₂ + O₂						
Hydroxyl + Ozone						
73 AND/KAU2	EX	220-450	7.83(11)	0	956	2
73 DEM	EX	300	4.81(10)			2
73 KUR	EX	298	(3.91±0.60)(10)			2
74 SIM/HEI1	ES	298	≥9.03(9)			2
Lower-limit k.						
74 SIM/HEI1	ES	298	(3.01±1.81)(10)			2
75 DEM	RL	271-333	1.68(1)	0	1233	2/2
k _{ref} : CO + OH → CO ₂ + H.						
75 DEM	RN	271-333	1.51(12)	0	1233	2
Estimated k.						
78 CHA/KAU	ES	295	(3.76±0.15)(10)			2
Laser-induced fluorescence technique.						
79 RAV/WIN1	EX	238-357	(1.10±0.21)(12)	0	930±50	2
Flash-photolysis. Resonance-fluorescence.						
See RAV/WIN2 for erratum.						
80 ZAH/HOW	RN	300	(3.91±0.60)(9)			2
Discharge-flow. Laser Magnetic Resonance.						
OH(v=n) + O₃ → HO₂ + O₂ (a)						
→ OH + O + O ₂ (b)						
→ H + O ₂ + O ₂ (c)						
Hydroxyl + Ozone						
71 COL/WOR ¹⁾	EX	298	(1.14±0.66)(12)			2
v = 2.						
71 COL/WOR ¹⁾	EX	298	(4.64±0.18)(12)			2
v = 9.						
¹⁾ k _a + k _b + k _c .						
71 POT/COL	EX	298	(4.64±0.18)(12)			2
k _a + k _b + k _c . v = 9.						
76 STR/JOH ¹⁾	EX	300	(2.23±0.06)(12)			2
v = 4.						
76 STR/JOH ¹⁾	EX	300	(6.63±2.41)(12)			2
v = 9.						
¹⁾ k _a + k _b + k _c .						
OD(v=n) + O₃ → DO₂ + O₂ (a)						
→ OD + O + O ₂ (b)						
→ D + O ₂ + O ₂ (c)						
Hydroxyl-d + Ozone						
74 BAS/ORA	EX	298	(3.31±0.54)(12)			2
k _a + k _b + k _c .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
OH + H₂ → H₂O + H							
Hydroxyl + Hydrogen molecule							
71 BRA/BEL1	EX	1100-1600	2.1(13)	0	2567±151	2	2.57
71 EBE/HOY	DE	500-1600	1.0(13)	0	2416	2	
72 DIX ¹⁾	RL	1050	(1.13±0.70)(1)			2/2	
k _{ref} : OH + CO → CO ₂ + H.							
72 DIX ¹⁾	RL	298-1330	(1.20±0.15)(2)	0	2400±50	2/2	
k _{ref} : OH + CO → CO ₂ + H.							
Combination of present and other data.							
72 DIX ¹⁾	ES	1050	(2.7±0.4)(12)			2	
72 DIX ¹⁾	SE	298-1330	3.72(13)	0	2770±100	2	
Combination of present and other data.							
¹⁾ Fuel-rich H ₂ /N ₂ /O ₂ flames.							
72 STU/NIK1	EX	298	4.28(9)			2	1.15
73 DAY/THO	ES	1050	(2.7±0.4)(12)			2	
73 DAY/THO	RL	298-1330	(1.20±0.15)(2)	0	2400±50	2/2	
Estimated ratio.							
73 GAR/MAL	EX	1200-2500	5.2(13)	0	3271	2	1.20
73 SMI/ZEL2	EX	210-460	1.4(13)	0	2416	2	
73 WES/DEH1	EX	298-745	4.6(9)			2	
Non-linear Arrhenius behavior.							
Within the given T-range, k increases							
k increases from 4.6x10 ⁹ to							
4.0x10 ¹¹ cm ³ mol ⁻¹ s ⁻¹ .							
74 GAR/MAL	EX	1350-1600	5.2(13)	0	3248	2	
74 GAR/MAL	SE	300-1800	7.57(11)	1.77	1528	2	
Combination of present and other data.							
The preexponential factor expressed							
as: A(T/298) ^{1.77} .							
74 SMI/ZEL	EX	298	(4.28±0.06)(9)			2	
74 SMI/ZEL	EX	210-460	(1.08±0.54)(13)	0	2334±120	2	
75 ATK/HAN1	EX	298	(4.20±0.42)(9)			2	
75 ATK/HAN2	EX	297-434	3.55(12)	0	2008±151	2	
75 ATK/HAN2	EX	298	(4.20±0.42)(9)			2	
75 OVE/PAR	EX	295	(3.49±0.16)(9)			2	
75 TRA/ROS	EX	300	3.91(9)			2	
H ₂ O is vibrationally excited.							
75 VAN/PEE	EX	600-1300	7.0(12)	0	2214	2	
76 BRA/CAP	RL	1300	5.9(-1)			2	
k _{ref} : OH + CH ₄ → H ₂ O + CH ₃							
77 SHA	ES	250-2000	1.33(12)	0.75	1575	2	
The preexponential factor expressed							
as: A(T/298) ^{0.75} .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 BIE/ZET2 M = He. Pulsed vacuum UV-Photolysis. Resonance-absorption. P(He) = 740 torr.	EX	297	(4.3±0.5)(9)			2	
78 PRE Laser Magnetic Resonance Spectrometry.	EX	293	(2.6±0.7)(9)			2	
79 COH/WES Critical review. The preexponential factor expressed as: $A(T/298)^{1.3}$. Alog k = 0.1 at 300 K, 0.15 for the (250-500) K range, and 0.3 at 2000 K.	RE	250-3000	1.81(12)	1.3	1835	2	
79 ZEL Critical evaluation. Best fit of all available experimental data. The preexponential factor expressed as: $A(T/298)^{1.6}$.	SE	300-2000	9.09(11)	1.6	1660	2	
80 SWO/HOC Flash-photolysis of H ₂ O vapor. P ~ 760 torr.	EX	296	(5.1±1.1)(9)			2	
80 TUL/RAV M = Ar. Flash-photolysis. Resonance-fluorescence. Non-linear, best-fit Arrhenius expression. The preexponential factor expressed as: $A(T/298)^{2.44}$. P(H ₂) = (0-1) torr. P(H ₂ O) = 150 torr. P(Ar) = 50 torr.	EX	298-992	2.70(11)	2.44	1281	2	
81 RAV/NIC M = Ar. Flash-photolysis of H ₂ /H ₂ O/Ar mixtures. Resonance-fluorescence. Low-T, linear Arrhenius expression. P(Ar) ~ 100 torr.	EX	250-400	(2.95±0.30)(12)	0	1990±340	2	
OH(v=1) + H₂ → H₂O + H							
Hydroxyl + Hydrogen molecule							
77 SPE/END Upper-limit k.	EX	295	<6.02(9)			2	
OH(v=n) + H₂(v=1) → H₂O + H							
Hydroxyl + Hydrogen molecule							
78 LIG/MAT n = 0. Flow-tube with tunable dye laser. Upper-limit k.	EX	298	≤3.3(12)			2	
81 GLA/CHA n = 0. Discharge-flow system. OH produced by reacting H with NO ₂ . EPR-spectroscopy. P(H ₂) = (1-2) torr.	EX	296	(6.0±1.5)(11)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 ZEL/STE n = 0. H ₂ (v=1) generated in a flow system by passing H ₂ over a heated W filament. OH enenerated by reacting H with NO ₂ . Resonance-fluorescence. [H ₂ (v=1)] = (0.562.70)x10 ¹⁴ molec.cm ³ . [OH] ₀ = 4.9x10 ¹² molec.cm ⁻³ . [H ₂] ~ 5.010 ¹⁶ molec.cm ⁻³ .	EX	298	(4.5±1.8)(11)			2
78 LIG/MAT n = 1. Flow-tube with tunable dye laser. Upper-limit k.	EX	298	≤5.7(12)			2
OH + HD → HDO + H						
Hydroxyl + Deuterium hydride						
72 DIX ¹⁾ k _{ref} : OH + HD → HOD + H.	RL	1050	(2.8±0.42)			2/2
72 DIX ¹⁾ k _{ref} : OH + HD → HOD + H. Estimated ratio.	RL	1050	2.4	0	-155	2/2
72 DIX ¹⁾ ¹⁾ Fuel-rich H ₂ /N ₂ /O ₂ flames.	ES	1050	(9.6±0.5)(11)			2
73 DAY/THO	ES	1050	(9.6±0.5)(11)			2
OH + D₂ → HDO + D						
Hydroxyl + Deuterium molecule						
72 STU/NIK1	EX	298	1.153(9)			2 1.15
74 SMI/ZEL	EX	298	(1.33±0.24)(9)			2
74 SMI/ZEL	EX	210-460	(7.53±0.36)(12)	0	2586±180	2
80 PAR/NIP Flash-photolysis. Resonance-absorption.	EX	297	(1.27±0.11)(9)			2
81 RAV/NIC ¹⁾ M = Ar. Non-linear Arrhenius expression over the whole T-range. The preexponential factor expressed as: A(T/298) ^{1.18} .	EX	250-1050	2.19(12)	1.18	2332	2
81 RAV/NIC ¹⁾ M = Ar. n = 0 assumed. Low T-range. ¹⁾ Flash-photolysis of D ₂ /H ₂ O/Ar mixtures. Resonance-fluorescence. P(Ar) ~100 torr.	EX	250-470	(7.29±3.13)(12)	0	2670±150	2
OD + H₂ → HDO + H						
Hydroxyl-d + Hydrogen molecule						
80 PAR/NIP Flash-photolysis. Resonance-absorption.	EX	297	(3.70±0.25)(9)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
OD + D₂ → D₂O + D							
Hydroxyl-d + Deuterium molecule							
75 APP/APP Data-fit.	ES	1700-3100	6.63(13)	0	2592	2	3.02
80 PAR/NIP Flash-photolysis. Resonance-absorption.	EX	297	(1.33±0.13)(9)			2	
OH + OH (+ M) → H₂O + O (+ M) (a)							
→ HO ₂ + H (+ M) (b)							
→ H ₂ O ₂ (+ M) (c)							
Hydroxyl							
73 GAR/MAL ¹⁾	EX	1200-2500	5.5(13)	0	3523	2	1.25
73 MCK/MUL ¹⁾	EX	298	(1.3±0.3)(12)			2	
73 WES/DEH2 ¹⁾	EX	298	(1.4±0.2)(12)			2	
¹⁾ k _a .							
74 CLY/DOW ²⁾	EX	300	(1.02±0.36)(12)			2	
74 CLY/DOW ²⁾	SE	300	(8.43±1.20)(11)			2	
k based on present and previous data.							
²⁾ k _a . Discharge-flow. Resonance-fluorescence.							
74 RAW/GAR2 ³⁾	RN	1200-2000	5.5(13)	0	3488	2	
n = 0 assumed.							
74 RAW/GAR2 ³⁾	CO	1200-2000	1.19(12)	1.11	0	2	
Data fit. B = 0 assumed.							
The preexponential factor expressed as: A(T/298) ^{1.11} .							
74 RAW/GAR2 ³⁾	CO	1200-2000	1.77(11)	2.03	-600	2	
Data fit. The preexponential factor expressed as: A(T/298) ^{2.03} .							
³⁾ k _a .							
74 TRA/ROS1	EX	298	(1.26±0.12)(12)			2	
k _a . H ₂ O is vibrationally excited.							
77 ERN/WAG ⁴⁾	EX	1180-1820	3.4(13)	0	2526	2	
77 ERN/WAG ⁴⁾	SE	300-2000	9.92(11)	1.14	0	2	
Modified Arrhenius expression based on weighed absolute values of all available data.							
77 ERN/WAG ⁴⁾	CO	300-2000	7.29(11)	1.23	0	2	
Modified Arrhenius expression.							
Transition-State Theory calculation.							
E _a = 0 at 300 K and ~2400 calmol ⁻¹ in the (1000-2000) K range.							
⁴⁾ k _a . Shock heating of HONO ₂ /Ar mixtures. The preexponential factor expressed as: A(T/298) ⁿ in the modified Arrhenius expressions.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 SHA k _a . The preexponential factor expressed as: A(T/298) ^{0.75} .	ES	250-2000	1.33(12)	0.75	0	2	
79 ZEL k _a . 5) k = exp(27.1 + 1.5x10 ⁻³ T) cm ³ mol ⁻¹ s ⁻¹ Critical evaluation. Non-Arrhenius best-fit of all available experimental data.	SE	300-2000	5)	5)	5)	2	
80 FAR/SMI k _a . Discharge flow. Resonance-fluorescence.	EX	298	(1.02±0.12)(12)			2	
81 WAG/ZEL k _a . Alternative non-Arrhenius expression over the extended T-range (250-2000) K: k = 6.02x10 ²³ exp(-27.73 + 1.49x10 ⁻³ T) cm ³ mol ⁻¹ s ⁻¹ . Flash-photolysis of H ₂ O/N ₂ mixtures. UV-Resonance spectrometry. P < 100 torr.	EX	250-580	(1.93±0.48)(12)	0	242	2	
79 HAC/PRE1 k _b . Isothermal flow-reactor. Laser Magnetic Resonance. k ₁ = k ₋₁ K. P(Total) = (130-800) Pa.	DE	298	1.1(-16)			2	
74 TRA/ROS1 k _c . M = N ₂ .	EX	298	(9.07±1.09)(16)			3	
OH + HO ₂ → H ₂ O + O ₂							
Hydroxyl + Hydroperoxo							
72 DAY/DIX k _{ref} : H + HO ₂ → H ₂ + O ₂ . Upper-limit ratio.	RL	300-1800	≤5.5			2/2	
72 FRI/SUT	ES	2130	1.2(13)			2	
72 HOC/GHO	EX	298	(1.2±0.2)(14)			2	
73 DAY/THO k _{ref} : H + HO ₂ → H ₂ + O ₂ . Upper-limit ratio.	RL	300-1050	≤5.5			2/2	
73 PEE/MAH1	ES	1600	≈5.0(13)			2	
74 DEM/TSC	ES	298	9.64(13)			2	3.0
75 GLA/TRO Upper-limit k.	EX	1350-1700	≤4.0(13)			2	
75 HAC/HOY Upper-limit k.	EX	298-670	≤2.0(13)			2	
77 BUR/HAR	EX	293	(3.07±0.96)(13)			2	
78 CHA/KAU Discharge-flow. Best fit between experiments and computer calculations.	DE	295	(1.5±0.3)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
78 COX Photolysis of $\text{Cl}_2/\text{H}_2/\text{NO}_2$ in N_2/O_2 . P = 1 atm.	ES	283	(9.03±0.30)(12)			2
78 HAC/PRE Isothermal discharge-flow. P(He) = 1.9 torr.	EX	293	(1.8±0.6)(13)			2
78 PRE Laser Magnetic Resonance Spectrometry.	EX	293	(1.8±0.6)(13)			2
79 BUR/CLI Discharge-flow.	EX	298	(3.07±1.02)(13)			2
79 DEM Photolysis of $\text{H}_2/\text{O}_2/\text{O}_3$ (or N_2) mixtures. Average of six reported k values.	RN	298	(9.8±2.4)(13)			2
80 HOC/SWO2 H_2O flash-photolysis in presence of O_2 and CO (or He). P = 760 torr.	EX	296	(7.0±1.5)(13)			2
80 LII/GOR2 Electron pulse-radiolysis. Kinetic Spectrophotometry. P(Total) = 1200 torr.	EX	308	(5.96±0.72)(13)			2
80 TEM/WAG Discharge-flow. Laser Magnetic Resonance.	EX	296	(3.9±1.5)(13)			2
81 BUR/COX Photolysis $\text{O}_3/\text{H}_2\text{O}/\text{O}_2$ mixtures in presence of N_2 or He. Molecular Modulation. T-independent in the given T-range. P(Total) = 760 torr.	DE	288-348	(3.73±2.41)(13)	0	0	2
81 COX/BUR Low-frequency square-wave modulated Photolysis of $\text{O}_3/\text{H}_2\text{O}$ mixtures. P = 760 torr.	EX	308	(6.0±1.5)(13)			2
81 KEY Discharge-flow Resonance-fluorescence. Mass-spectrometry. P(Total) = 1 torr.	EX	299	(3.9±0.9)(13)			2
81 SRI/QIU HO_2 produced by reacting F with H_2O_2 . Discharge-flow. Laser-induced Fluorescence. Resonance-fluorescence. P ~3 torr. [H_2O_2] ~ (6-26) × 10 ¹² molec.cm ⁻³ . [HO_2] ~ (2-19) × 10 ¹¹ molec.cm ⁻³ . [OH] ₀ = (4-6) × 10 ¹⁰ molec.cm ⁻³ . [H_2O] ~ 5 × 10 ¹³ molec.cm ⁻³ . [F ₂] ~ 6 × 10 ¹³ molec.cm ⁻³ .	EX	296	(4.5±0.7)(13)			2
81 THR/WIL1 Laser magnetic resonance spectrometry.	EX	298	(3.5±0.5)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 BRA/HOF H ₂ O flash-photolysis in N ₂ , with or without O ₂ . P(H ₂ O) = (0.2-2.1) torr. P(Total) = 750 torr. P(N ₂) = (728-984) torr. P(O ₂) = (0-17) torr.	ES	298	6.6(13)			2 1.3
82 DEM H ₂ O photolysis with O ₂ in traces. Laser-induced fluorescence. P(Total) = (75-730) torr. He, or Ar.	EX	298	(7.2±2.4)(13)			2
82 TEM/WAG1 Reaction of OH with HO ₂ in several isothermal discharge-flow-reactors. OH generated by reacting F with H ₂ O. HO ₂ generated by reacting OH with H ₂ O ₂ . [OH] ₀ = (1.93-3.79)×10 ¹² molec.cm ⁻³ . [H ₂ O ₂] = (0.36-4.82)×10 ¹³ molec.cm ⁻³ . P = (1.5-10.5) torr. k is independent within this P-range.	EX	296	(4.0±1.4)(13)			2
OH(v=9) + H ₂ O → products						
Hydroxyl + Water						
72 WOR/COL Lower-limit k. Unreported T assumed to be 298 K.	EX	298	≥1.20(11)			2
OH + H ₂ O ₂ → HO ₂ + H ₂ O						
Hydroxyl + Hydrogen peroxide						
72 GOR/VOL	EX	298	(7.23±0.18)(11)			2
72 VOL/GOR	EX	298	(7.23±0.18)(11)			2
73 GOR	RN	298	(7.47±0.48)(11)			2
74 HAC/HOY2	EX	298-669	(4.8±1.0)(12)	0	670±70	2
75 HAC/HOY	EX	298-670	(4.8±1.0)(12)	0	670±70	2
75 MEA/HEI k _{ref} : OH + CO → H + CO ₂	RL	298	(4.1±0.6)			2/2
78 PRE Laser Magnetic Resonance Spectrometry.	EX	293	(4.8±1.0)(11)			2
79 HAR/PIT Flash-photolysis. Resonance-fluorescence.	EX	298	(4.1±0.8)(11)			2
80 KEY Discharge-flow. Resonance-fluorescence. P(Total) = (1-4) torr.	EX	245-423	(1.5±0.4)(12)	0	126±76	2
80 SRI/REI Discharge-flow. Laser-induced fluorescence. [H ₂ O ₂] = (0.6-5.0)×10 ¹³ molec.cm ⁻³ . P(He) = (2-3) torr.	EX	250-459	(1.8±0.3)(12)	0	164±52	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
80 TEM/WAG Discharge-flow. Laser Magnetic Resonance.	EX	296	(1.05±0.20)(12)			2	
81 NEL/MAR M = Ar. Flash-photolysis combined with: either Resonance-fluorescence [P(Total) = 10-50 torr.], or Laser absorption [P(Total) = 10 torr.]	EX	295	(9.46±0.60)(11)			2	
81 WIN/SEM ¹⁾	EX	273-410	(2.23±0.36)(12)	0	260±50	2	
81 WIN/SEM ¹⁾ Average k of 80 KEY, 80 SRI/REI and 81 WIN/SEM data.	SE	273-410	(1.70±0.18)(12)	0	167±35	2	
¹⁾ Flash-photolysis of H ₂ O ₂ in He, or SF ₆ . Resonance-fluorescence. P(Total) = 100 torr. He, or 40 torr. SF ₆ . [H ₂ O ₂] = (0.36-3.60)×10 ¹⁵ molec.cm ⁻³ .							
82 KUR/MUR Flash-photolysis. Resonance-fluorescence. OH generated by Flash-photolysis of H ₂ O ₂ /Ar mix- tures. [H ₂ O] ~ 100 mtorr. [Ar] = (20-30) torr. [H ₂ O ₂] = (0-20) mtorr.	EX	250-370	(1.75±0.18)(12)	0	161±32	2	
82 MAR/JOH Flash-photolysis. Resonance-fluorescence. OH generated by Flash-photolysis of H ₂ O ₂ . P(Ar) = 10 torr.	EX	298	(1.9±0.14)(12)			2	
82 MOL/MOL Flash-photolysis. Resonance-fluorescence. UV-, and IR-spectrophotometry. P = 760 torr.	EX	294	(1.08±0.18)(12)			2	
82 TEM/WAG1 Reaction of OH with H ₂ O ₂ in several isothermal discharge-flow reactors. OH generated by reacting F with H ₂ O. P = (1.5-10.5) torr. k is P-independent within this P-range. [OH] ₀ = (0.57-2.59)×10 ¹¹ molec.cm ⁻³ . [H ₂ O ₂] = (0.36-6.02)×10 ¹³ molec.cm ⁻³ .	EX	296	(1.0±0.2)(12)			2	
OH + S → H + SO Hydroxyl + Sulfur atom							
79 JOU/LEB2 Discharge-flow reactor. EPR-spectrometer.	EX	298	(3.98±0.84)(13)			2	
OH + SO → H + SO ₂ Hydroxyl + Sulfur monoxide							
79 JOU/LEB2 Discharge-flow reactor. EPR-spectrometer.	EX	298	(5.06±0.90)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + SO₂ (+ M) → HOSO₂ (+ M)						
Hydroxyl + Sulfur dioxide						
74 COX2 Expressed as k[M], with M = N ₂ + O ₂ at 1 atm.	RN	294	(3.61±0.48)(11)			2
75 CAS/DAV Pseudo-second order k. M = N ₂ . Limiting high-pressure k. P = 760 torr.	EX	298	3.6(11)			2
75 COX Expressed as k[M], with M = N ₂ + O ₂ at 1 atm.	RN	300	(3.61±0.48)(11)			2
75 GOR/MUL1 M = He. In an atmosphere of Water vapor.	EX	435	(1.08±0.05)(12)			2
76 ATK/PER3 M = Ar. P = 760 torr.	EX	298	(4.04±0.42)(11)			2
76 ATK/PER3 M = Ar. Limiting high-pressure k.	ES	298	≈5.00(11)			2
77 CAS/TAN M = N ₂ . Limiting high-pressure k. P = 760 torr.	EX	297	3.61(11)			2
77 CAS/TAN The product is vibrationally excited.	EX	297	4.28(11)			2
79 DAV/RAV M = N ₂ . Flash-photolysis. Resonance-fluorescence. P = 760 torr. High-pressure k.	EX	298	5.42(11)			2
80 COX/SHE ¹⁾ k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	297	(9.0±2.0)(-2)			2/2
80 COX/SHE ¹⁾ ¹⁾ Photolysis of HONO and SO ₂ . Gas-chromatography. P = 760 torr.	RN	297	(4.34±0.96)(11)			2
80 HAR/ATK ²⁾ M = Ar.	EX	298-424	6.99(9)	0	-1193±151	2
80 HAR/ATK ²⁾ M = Ar.	EX	298	(3.91±0.51)(11)			2
80 HAR/ATK ²⁾ M = SF ₆ .	EX	298-424	7.65(10)	0	-752±151	2
80 HAR/ATK ²⁾ M = SF ₆ .	EX	298	(9.70±1.33)(11)			2
80 HAR/ATK ²⁾ M = N ₂ .	ES	298-424	2.41(10)	0	-956	2
80 HAR/ATK ²⁾ M = N ₂ .	ES	298	6.02(11)			2
²⁾ Flash-photolysis. Resonance-fluorescence. P(Total) ~ 650 torr. High-pressure k's.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
73 PAY/STI M = N ₂ (18 torr.) + H ₂ O(20 torr.)	RN	300	5.44(16)				3
75 CAS/DAV M = N ₂ . Low-pressure k. P < 20 torr.	EX	298	5.80(16)				3
75 HAR/WAY M = N ₂ . M-efficiencies relative to N ₂ are: 1.0(N ₂), 0.63(Ar).	EX	298	(2.61±0.94)(17)				3
76 ATK/PER3 M = Ar. Limiting low-pressure k.	EX	298	(5.95±1.20)(16)				3
77 CAS/TAN M = N ₂ . Low-pressure k.	EX	297	5.80(16)				3
77 CAS/TAN Low-pressure k. Expression based on the experimental values k(297) and E _a . n = 0 assumed.	EX	253-297	5.05(14)	0	-1409		3
77 CAS/TAN Low-pressure k. The preexponential factor expressed as: A(T/298) ^{-5.1} .	EX	253-297	6.11(16)	-5.1	0		3
82 LEU ³⁾ M = He. n = 0 assumed.	EX	261-414	(1.31±0.36)(15)	0	-913±74		3
82 LEU ³⁾ M = He. P = (0.9-10.0) torr.	EX	261-414	(2.87±0.09)(16)	-2.85	0		3
82 LEU ³⁾ M = Ar. P = (1.0-3.6) torr.	EX	298	(3.95±0.33)(16)				3
82 LEU ³⁾ M = N ₂ . P = (0.9-4.0) torr.	EX	298	(9.21±1.20)(16)				3
82 LEU ³⁾ M = O ₂ . P = (1.7-2.3) torr.	EX	298	(8.92±1.16)(16)				3
82 LEU ³⁾ M = CO ₂ . P = (0.6-1.7) torr.	EX	298	(4.35±1.12)(17)				3
82 LEU ³⁾ M = SO ₂ . n = 0 assumed.	EX	261-414	(1.93±0.98)(16)	0	-908±129		3
82 LEU ³⁾ M = SO ₂ . P = (0.02-0.20) torr.	EX	261-414	(4.17±0.33)(17)	-2.78	0		3
³⁾ Discharge-flow. Resonance-fluorescence. OH generated by reacting H with NO ₂ . Low-pressure k's. The preexponential factors expressed as: A(T/298) ⁿ . [OH] ₀ = (1.0-5.0)×10 ¹¹ molec.cm ⁻³ .							
OH(v=9) + SO ₂ → HOSO ₂ Hydroxyl + Sulfur dioxide							
72 WOR/COL Lower-limit k. Unreported T assumed to be 298 K.	EX	298	≥1.45(10)				2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
OH + H₂S → H₂O + SH							
Hydroxyl + Hydrogen sulfide							
72 NIK/MOR1	ES	300	~5.12(12)				2
73 WES/DEH3	EX	298-885	1.4(13)	0	443		2
73 WES/DEH3	EX	298	(3.3±0.2)(12)				2
74 STU2	EX	298	(1.87±0.30)(12)				2
76 PER/ATK1	EX	297-427	(3.13±0.30)(12)	0	0		2
76 PER/ATK1	EX	298	(3.16±0.32)(12)				2
80 COX/SHE ¹⁾	RL	297	(6.2±0.4)(-1)				2/2
k _{ref} : OH + CH ₂ =CH ₂ → products.							
80 COX/SHE ¹⁾	RN	297	(3.01±0.18)(12)				2
¹⁾ HONO/H ₂ S photolysis. P = 760 torr.							
81 WIN/KRE	EX	244-367	(3.85±0.78)(12)	0	55±58		2
Flash-photolysis of H ₂ O/Ar/H ₂ S mixtures. Resonance-fluorescence. P(Ar) = (40-120) torr. P(H ₂ O) = (0.05-0.19) torr.							
82 LEU/SMI1 ²⁾	EX	228-518	(3.55±0.36)(12)	0	89		2
n = 0 assumed.							
82 LEU/SMI1 ²⁾	EX	228-518	(2.16±0.15)(11)	2.5	-725		2
The preexponential factor expressed as: A(T/298) ^{2.5} .							
²⁾ Discharge-flow. Resonance-fluorescence. Mass-spectrometry. OH generated by reacting H with NO ₂ . [OH] ₀ = (0.6-4.0) × 10 ¹¹ molec.cm ⁻³ .							
82 LIN	EX	239-425	(4.70±1.57)(12)	0	146±105		2
Flash-photolysis. Resonance-fluorescence. OH generated by UV-photolysis of H ₂ O near 308 nm.							
82 MIC/NAV ³⁾	EX	228	(3.08±0.23)(12)				2
82 MIC/NAV ³⁾	EX	298	(2.66±0.22)(12)				2
82 MIC/NAV ³⁾	EX	437	(3.35±0.29)(12)				2
82 MIC/NAV ³⁾	EX	228-437	(3.01±0.33)(12)	0	0		2
Average value.							
³⁾ Reaction of H ₂ S with OH in Ar. Flash-photolysis. Resonance-fluorescence. OH generated by Flash-photolysis of H ₂ O. P(Ar) = (20-120) torr. P(H ₂ S) = (0.8-8.0) mtorr. P(H ₂ O) = (32-238) mtorr.							
OH(v=9) + H₂S → products							
Hydroxyl + Hydrogen sulfide							
72 WOR/COL	EX	298	≥1.51(11)				2
Lower limit k. Unreported T assumed to be 298 K.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + N₂ → H + N₂O						
Hydroxyl + Nitrogen molecule						
75 ALB/HOY k obtained from k ₋₁ and thermodynamic data.	DE	700-1100	3.2(12)	0	40512	2
OH(v=9) + N₂ → products						
Hydroxyl + Nitrogen molecule						
72 WOR/COL	EX	298	(2.17±0.30)(9)			2
OH + NO (+ M) → HONO (+ M)						
Hydroxyl + Nitrogen oxide (NO)						
72 STU/NIK2 M = He. Limiting high-pressure k.	EX	300	(1.20±0.60)(12)			2
74 COX2 M = N ₂ + O ₂ . P = 1 atm. k expressed as k[M].	RN	294	(3.67±0.66)(12)			2
75 ATK/HAN1 M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.85(Ar). P = 760 torr.	EX	298	(3.67±0.60)(12)			2
75 ATK/HAN1 Extrapolated limiting high-pressure k.	ES	298	4.81(12)			2
75 COX M = N ₂ + O ₂ . P = 1 atm. k expressed as k[M].	RN	300	(3.67±0.78)(12)			2
75 GOR/MUL1 M = H ₂ O. In an atmosphere of water vapor.	EX	435	(4.5±0.2)(12)			2
76 BLA/OVE M = H ₂ O. M-efficiencies relative to H ₂ O are: 1.00(H ₂ O), 0.02(He), 0.12(N ₂), 0.37(SF ₆), 0.41(CF ₄). Flash-photolysis. Resonance-absorption. Limiting high-pressure k.	EX	295	(1.1±0.1)(13)			2
76 COX/DER1 k _{ref} : OH + H ₂ → H ₂ O + H. M = N ₂ + O ₂ . P = 1 atm.	RL	298	(1.63±0.24)(3)			2/2
76 COX/DER1 M = N ₂ + O ₂ .	RN	298	(7.05±1.02)(12)			2
76 OVE/PAR M = H ₂ O, CF ₄ , SF ₆ , N ₂ , Ar, or He. Limiting high-pressure k. The product is vibrationally excited.	EX	295	(1.11±0.10)(12)			2
76 SIE/SIM2 M = 80% H ₂ , (18-20)% N ₂ O, (1-2)% CO. k _{ref} : OH + CO → H + CO ₂ . P = (408-768) torr.	RL	298	(2.2±0.3)(1)			2/2
76 SIE/SIM2 M = 63% H ₂ , 30% N ₂ O, 7% CO. P = 96 torr. k _{ref} : OH + CO → H + CO ₂ .	RL	298	(1.61±0.2)(1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
76 SIE/SIM2 Limiting high-pressure k.	RN	298	7.23(12)			2	
76 SIM/HEI $k_{\text{ref}}: \text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}.$	RL	296	(4.83±0.50)(2)			2/2	
76 SIM/HEI M = H ₂ . P ~ 100 torr.	ES	296	2.23(12)			2	
76 SIM/HEI M = H ₂ . P ~ 730 torr.	ES	296	6.63(12)			2	
78 ANA/SMI1 ¹⁾	EX	233	7.83(12)			2	
78 ANA/SMI1 ¹⁾	EX	296	4.04(12)			2	
78 ANA/SMI1 ¹⁾	EX	298	5.12(12)			2	
78 ANA/SMI1 ¹⁾	EX	405	6.63(12)			2	
78 ANA/SMI1 ¹⁾	EX	505	4.22(12)			2	
¹⁾ Flash-photolysis. Resonance-absorption. High-pressure k. P = 1 atm.							
79 CAM/PAR Boric-acid-coated Pyrex reaction vessels. P = 100 torr.	EX	292	(8.2±1.2)(11)			2	
72 AND/KAU M = Ar. P = 5 torr.	EX	297	(1.45±0.73)(17)			3	
72 AND/KAU M = Ar. P = 8 torr.	EX	297	(9.07±0.36)(16)			3	
72 MOR/SMI M = He. Low-pressure k.	EX	300	(1.49±0.22)(12)			3	
72 MOR/SMI M = He. Low-pressure k.	EX	416	6.89(16)			3	
72 MOR/SMI M = He. Low-pressure k. Based on the given E _a and the experimental k's at 300 K and 416 K.	CO	300-416	1.00(16)	0	-806±241	3	
72 WES/DEH4 M = He. k decreasing within the given T-range from 4.7x10 ¹⁷ to 1.3x10 ¹⁷ cm ⁶ mol ⁻¹ s ⁻¹ .	EX	273-395	4.7(17)			3	
72 WES/DEH4 M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 2.23(He).	EX	298	1.3(17)			3	
74 AND/MAR M = He.	EX	230-450	6.58(15)	0	-856±151	3	1.2
74 AND/MAR M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.57(He), 0.59(Ar). P(Ar) = (1-10) torr. P(He) = (1-10) torr. P(N ₂) = (2-5) torr.	EX	295	(2.10±0.44)(17)			3	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
74 HOW/EVE M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.51(He), 0.56(Ar).	EX	296	2.83(17)			3
75 ATK/HAN1 M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.70(Ar). Low-pressure k.	EX	298	(2.21±0.25)(17)			3
75 HAR/WAY M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.47(Ar).	EX	298	(5.44±1.81)(17)			3
78 ANA/SMI1 ²) M = N ₂ . Limiting low-pressure k.	EX	233	4.17(17)			3
78 ANA/SMI1 ²) M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.37(He), 0.50(Ar). Limiting low-pressure k.	EX	296	2.97(17)			3
78 ANA/SMI1 ²) M = N ₂ . Limiting low-pressure k.	EX	405	1.05(17)			3
78 ANA/SMI1 ²) M = N ₂ . Limiting low-pressure k. ²) Flash-photolysis. Resonance-absorption.	EX	505	8.71(17)			3
OH(v=9) + NO → HONO						
Hydroxyl + Nitrogen oxide (NO)						
72 WOR/COL	EX	298	(9.03±1.81)(10)			2
OH + NO ₂ (+ M) → HO ₂ + NO (+ M) (a) → HONO ₂ (+ M) (b)						
Hydroxyl + Nitrogen oxide (NO ₂)						
75 GLA/TRO k _a . Increasing to 1.9x10 ¹² cm ³ mol ⁻¹ s ⁻¹ at 1700 K.	ES	1350	≈7.0(11)			2
80 HOW k _a . Discharge-flow. Laser Magnetic Resonance.	EX	452-1115	(1.82±0.36)(13)	0	3360±135	2
72 SIM/HEI2 k _b . M = H ₂ O. Limiting high-pressure k.	RN	300-423	6.3(12)	0	171	2
74 GLA/TRO1 k _b . M = Ar. Limiting high-pressure k. The preexponential factor expressed as: A(T/298) ^{-0.85} . k ₁ k ₋₁ K.	DE	295-1200	3.14(12)	-0.85	0	2 1.58
75 GOR/MUL1 k _b . M = H ₂ O. IN an atmosphere of water vapor.	EX	435	3.2(12)			2
76 ANA/SMI k _b . M = N ₂ . Limiting high-pressure k.	EX	296	9.78(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 ATK/PER3 k_b . M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.92(Ar). P = 760 torr.	EX	298	(3.85±0.60)(12)			2
76 ATK/PER3 k_b . M = Ar, or N ₂ . Limiting high-pressure k.	ES	298	≈5.12(12)			2
78 ANA/SMI3 ¹⁾	EX	220	1.20(13)			2
78 ANA/SMI3 ¹⁾	EX	296	9.64(12)			2
78 ANA/SMI3 ¹⁾	EX	358	7.83(12)			2
78 ANA/SMI3 ¹⁾	EX	450	2.29(12)			2
78 ANA/SMI3 ¹⁾	EX	550	2.65(12)			2
¹⁾ k_b . M = N ₂ . Flash-photolysis. Resonance-absorption. Limiting high-pressure k's.						
79 CAM/PAR ²⁾ k_b . M = CO. P = 100 torr.	EX	292	(2.5±0.4)(12)			2
79 CAM/PAR ²⁾ k_b . M = N ₂ . P = 5.49 torr.	EX	292	(1.2±0.3)(12)			2
²⁾ Boric-acid-coated Pyrex reaction vessels.						
79 O'B/GRE k_b . Photolysis of an Air/H ₂ O/NO _x mixture. P(Air) = 780 torr. P(H ₂ O) = 11 torr.	EX	301	(7.83±1.81)(12)			2
79 WIN/KRE ³⁾ [N ₂] = 5.4×10 ¹⁷ molec.cm ⁻³ . M-efficiencies relative to N ₂ are: 0.35(He), 0.55(Ar), 1.00(N ₂), 1.7(SF ₆).	EX	247	(1.10±0.09)(12)			2
79 WIN/KRE ³⁾ [N ₂] = 5.4×10 ¹⁷ molec.cm ⁻³ . M-efficiencies relative to N ₂ are: 0.45(He), 0.65(Ar), 1.00(N ₂), 2.6(SF ₆).	EX	297	(6.00±0.46)(11)			2
79 WIN/KRE ³⁾ P(N ₂) = 760 torr.	EX	297	6.63(12)			2
79 WIN/KRE ³⁾ [N ₂] = 5.4×10 ¹⁷ molec.cm ⁻³ . M-efficiencies relative to N ₂ are: 0.45(He), 0.60(Ar), 1.00(N ₂), 2.9(SF ₆).	EX	352	(4.10±0.30)(11)			2
³⁾ k_b . M = N ₂ . Flash-photolysis. Resonance-fluorescence. k values reported for different [M] up to 2.3×10 ¹⁹ molec.cm ³ , in the T-range (247-352) K.						
80 AND k_b . Limiting high-pressure k. The preexponential factor expressed as: A(T/298) ^{-1.6} . Discharge-flow. Resonance-fluorescence.	CO	220-1100	7.23(12)	-1.6	0	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A	k err. units factor
82 ROB/SMI k_b . Pulsed-photolysis of HONO_2 in Ar, or CF_4 . High-pressure k. $P(\text{Ar}) = 4$ atm. $P(\text{CF}_4) = 8.6$ atm. $[\text{N}_2] = 3.2 \times 10^{17} - 4.0 \times 10^{18}$ molec. cm^{-3} .	EX	295	$\approx 1.81(13)$			2	
72 AND/KAU k_b . M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 2.0(N_2).. Low-pressure k. $P(\text{Ar}) = 3$ torr. $P(\text{N}_2) = 8$ torr.	EX	297	$(3.63 \pm 1.09)(17)$			3	
72 SIM/HEI2 k_b . M = H_2O . Limiting low-pressure k.	RN	300-423	4.0(18)	0	0	3	
72 WES/DEH4 k_b . M = He. k decreasing within the given T-range from 7.3×10^{17} to 2.1×10^{17} $\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$.	EX	273-395	7.3(17)			3	
72 WES/DEH4 k_b . M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 1.9(He).	EX	298	3.0(17)			3	
74 AND/MAR k_b . M = Ar.	EX	230-450	1.68(16)	0	-906 $\pm$ 151	3	1.2
74 AND/MAR k_b . M = N_2 . M-efficiencies relative to N_2 are: 1.00(N_2), 0.43(He), 0.43(Ar). $P(\text{He}) = (1-10)$ torr. $P(\text{Ar}) = (1-10)$ torr. $P(\text{N}_2) = (1-8)$ torr.	EX	295	$(8.34 \pm 1.81)(17)$			3	
74 GLA/TRO1 ⁴⁾ k_b . M = He. Limiting low-pressure, concentra- tion-dependent expression = $k/[\text{He}]$. $k_1 = k_{-1}K$.	DE	295-1200	5.84(17)	-2.98	0	3	1.58
74 GLA/TRO1 ⁴⁾ k_b . M = Ar. Limiting low-pressure, concentra- tion-dependent expression = $k/[\text{Ar}]$. $k_1 = k_{-1}K$.	DE	295-1200	3.75(17)	-2.9	0	3	1.58
⁴⁾ The preexponential factors expressed as: $A(T/298)^n$.							
74 GLA/TRO1 k_b . M = N_2 . Limiting low-pressure, concentra- tion-dependent expression = $k/[\text{N}_2]$. $k_1 = k_{-1}K$.	DE	622	3.0(17)			3	
74 GLA/TRO1 k_b . M = N_2 . Limiting low-pressure, concentra- tion-dependent Arrhenius expression = $k/[\text{N}_2]$. Determined by using $k_1 = Kk_{-1}$.	DE	670	1.7(17)			3	
74 HOW/EVE k_b . M = N_2 .	EX	296	1.05(18)			3	
75 HAR/WAY k_b . M = N_2 . M-efficiencies relative to N_2 are: 1.00(N_2), 0.58(Ar).	EX	298	$(9.43 \pm 3.63)(17)$			3	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
76 ANA/BEM k_b . M = N ₂ . Resonance absorption. Limiting low-pressure k. k decreases from $2.0 \times 10^{18} \text{ cm}^6 \text{ mol}^{-2} \text{ s}^{-1}$ at T = 220K, to $5.9 \times 10^{17} \text{ cm}^6 \text{ mol}^{-2} \text{ s}^{-1}$ at T = 358K. [N ₂] = 3.2×10^{17} – $4.0 \times 10^{18} \text{ molec. cm}^{-3}$.	EX	220	1.96(18)			3
76 ANA/SMI k_b . M = N ₂ . Limiting low-pressure k. M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.34(He), 0.42(Ar), 0.68(O ₂), 2.53(SF ₆).	EX	296	9.43(17)			3
76 ANA/SMI k_b . M = N ₂ . Limiting low-pressure k. n = 0 assumed. A and B recalculated from the reported data.	EX	220-550	(5.26±1.78)(16)	0	-818±79	3
76 ANA/SMI k_b . M = N ₂ . Limiting low-pressure k. The A-factor recalculated from the reported experimental data. The preexponential factor expressed as: $A(T/298)^{-2.6}$.	EX	220-550	(9.67±2.18)(17)	-2.6	0	3
76 ATK/PER3 k_b . M = Ar. Limiting low-pressure k.	EX	298	(3.70±0.36)(17)			3
77 ERL/FIE k_b . M = He. Low pressure k. The preexponential factor expressed as: $A(T/298)^{-2.9}$.	EX	213-300	(3.60±0.97)(17)	-2.9	0	3
77 ERL/FIE k_b . M = He. Low-pressure k. M-efficiencies relative to He are: 1.00(He), 4.00(CO ₂).	EX	300	(3.63±1.45)(17)			3
78 ANA/SMI3 ⁵⁾ k_b . M = N ₂ .	EX	220	2.29(18)			3
78 ANA/SMI3 ⁵⁾ k_b . M = N ₂ .	EX	296	9.61(17)			3
78 ANA/SMI3 ⁵⁾ k_b . M = N ₂ .	EX	358	6.06(17)			3
78 ANA/SMI3 ⁵⁾ k_b . M = N ₂ .	EX	450	3.95(17)			3
78 ANA/SMI3 ⁵⁾ k_b . M = N ₂ .	EX	550	2.21(17)			3
78 ANA/SMI3 ⁵⁾ k_b . M = He.	EX	220	9.07(17)			3
78 ANA/SMI3 ⁵⁾ k_b . M = He.	EX	296	3.30(17)			3
⁵⁾ Flash-photolysis. Resonance-absorption. Limiting low-pressure k's.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
78 ANA/SMI3 ⁶) k _b . M = He.	EX	220	1.09(18)			3
78 ANA/SMI3 ⁶) k _b . M = He.	EX	296	3.81(17)			3
⁶) Discharge-flow. Resonance-fluorescence. Limiting low-pressure k's.						
80 AND ⁷) k _b . M = N ₂ . Limiting low-pressure k. P(N ₂) = (0.8-2.0) torr. n = 0 assumed.	EX	225-389	(5.80±1.45)(16)	0	-785±136	3
80 AND ⁷) k _b . The preexponential factor expressed as: A(T/298) ^{-2.9} . P(N ₂) = (0.8-2.0) torr.	EX	225-389	(8.34±2.18)(17)	-2.9	0	3
80 AND ⁷) k _b . M = He. Limiting low-pressure k. P(He) = (1.5-2.7) torr.	EX	298	(6.17±0.73)(17)			3
⁷) Discharge-flow. Resonance-fluorescence.						
OH + N ₂ O (+ M) → HO ₂ + N ₂ (+ M) (a) → products (b)						
Hydroxyl + Nitrogen oxide (N ₂ O)						
76 BIE/ZET k _a .	EX	298	(2.29±0.72)(7)			2
77 CHA/KAU k _a . Upper-limit k.	EX	480	≤2.41(8)			2
75 GOR/MUL1 k _b . M = H ₂ O. Upper-limit k. In an atmosphere of Water vapor.	EX	440	<1.0(10)			2
76 ATK/PER2 k _b . M = Ar. Limiting high-pressure, upper-limit k.	EX	298-443	≤1.20(8)			2
OH(v=9) + N ₂ O → products						
Hydroxyl + Nitrogen oxide (N ₂ O)						
72 WOR/COL	EX	298	(2.89±1.33)(10)			2
OH + NH ₂ → products						
Hydroxyl + Amidogen						
80 FEN Lean-burnt gas mixture. Average ratio. k _{ref} : NO + NH ₂ → N ₂ + H ₂ O.	RL	1110-1500	(1.0±0.5)(1)	0	0	2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + NH₃ → H₂O + NH₂						
Hydroxyl + Ammonia						
73 GEH/HOY	EX	298	1.7(11)			2
73 KUR	EX	298	(2.47±0.36)(10)			2
73 STU3	EX	298	(9.03±2.41)(10)			2
74 DOV/NIP	EX	1620-1920	≤3.85(11)	0.68	554	2
Upper-limit k. Preexponential factor expressed as: A(T/298) ^{0.68} .						
74 HAC/HOY1	EX	298-669	(3.2±0.5)(12)	0	920	2
74 HAC/HOY1	EX	298	(1.3±0.3)(13)			2
74 ZEL/SMI	EX	230-490	1.39(12)	0	805	2 1.07
74 ZEL/SMI	EX	298	9.52(10)			2
75 COX/DER2	ES	296	(7.23±2.41)(10)			2
75 GOR/MUL1	EX	418	(2.6±0.3)(11)			2
M = H ₂ O. In an atmosphere of Water vapor.						
75 SMI/ZEL	EX	228-472	1.39(12)	0	805	2 1.07
75 ZEL	EX	228-472	1.4(12)	0	800	2
Flash-photolysis. Resonance-absorption.						
76 PER/ATK1	EX	297-427	1.76(12)	0	861±151	2
76 PER/ATK1	EX	298	(9.88±0.96)(10)			2
79 PAG/ERI ¹⁾	EX	300	(1.6±0.2)(11)			2
79 PAG/ERI ¹⁾	EX	298-365	(6.89±0.86)(11)	0	438±40	2
Based on the experimental k at 300 K and the reported E _a .						
¹⁾ Gaseous NH ₃ pulse-radiolysis.						
80 FEN	ES	1235	3.0(11)			2
Lean-burnt gas mixture. Tentative k.						
80 SIL/KOL	EX	294-1075	(3.26±0.52)(12)	0	1067±72	2
Discharge-flow. Mass-spectrometry.						
81 FUJ/MIY1 ²⁾	SE	300-2200	3.16(12)	0	1007	2
Obtained by combining the present data with those reported in 74 HAC/HOY.						
81 FUJ/MIY2 ²⁾	EX	1360-1840	3.09(12)	0	981±75	2 1.1
²⁾ Oxidation of NH ₃ behind reflected shock-waves, in NH ₃ /H ₂ /O ₂ /Ar mixtures.						
81 NIE/WAG ³⁾	EX	300-1400	(2.5±1.0)(12)	0	980	2
n = 0 assumed.						
81 NIE/WAG ³⁾	EX	300-1400	3.15(11)	1.05	350	2
The preexponential factor expressed as: A(T/298) ^{1.05} .						
³⁾ OH radicals generated by H ₂ O photolysis at 165-185 nm. Shock-waves. Flash-photolysis.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + NH₂NH₂ → products						
Hydroxyl + Hydrazine						
74 HAC/HOY1	EX	298	1.3(13)			2 1.2
79 HAR/ATK ¹⁾ M = Ar. P(Ar) = (25-50) torr.	EX	298-424	2.65(13)	0	-116±176	2
79 HAR/ATK ¹⁾ B = 0 assumed.	EX	298-424	(3.67±0.60)(13)	0	0	2
¹⁾ Flash-photolysis. Resonance-fluorescence.						
OH + HNO → H₂O + NO						
Hydroxyl + Nitrosyl hydride						
72 SMI	EX	2100	(1.08±0.12)(13)			2
75 CAM/HAN2	RL	425	≤4.4			2/2
k _{ref} : O + HNO → H ₂ + NO. Upper-limit ratio.						
OH + HONO → H₂O + NO₂						
Hydroxyl + Nitrous acid						
74 COX1	RL	300	(3.7±0.6)(-1)			2/2
k _{ref} : OH + NO + M. → HONO + M.						
74 COX1	RN	300	1.08(12)			2
74 COX2	RN	294	(1.33±0.12)(12)			2
75 COX	RN	300	(1.33±0.12)(12)			2
75 COX/DER2	ES	296	2.17(12)			2
76 COX/DER1	RL	298	(9.45±0.48)(2)			2/2
k _{ref} : OH + H ₂ → H ₂ O + H.						
76 COX/DER1	RN	298	(3.98±0.18)(12)			2
76 COX/DER2	RL	298	(9.04±0.94)(2)			2/2
k _{ref} : OH + CH ₄ → H ₂ O + CH ₃ .						
76 COX/DER3	RL	296	(3.25±0.44)(-1)			2/2
k _{ref} : OH + CH ₃ CHO → H ₂ O + CH ₃ CO						
76 FIF	RN	1000-1400	(1.55±0.5)(12)	0	0	2
76 FIF	RN	1000-1400	6.92(12)	0	1761	2
B = 0 assumed.						
OH + HONO₂ → H₂O + NO₃ (a)						
→ H ₂ O ₂ + NO ₂ (b)						
→ [HO.HONO ₂] [†] (c)						
Hydroxyl + Nitric acid						
72 MOR/SMI ¹⁾	EX	300	(7.82±3.01)(10)			2
74 GLA/TRO1 ¹⁾	EX	1000-1100	(9.5±2.0)(10)	0	0	2
74 ZEL/SMI ¹⁾	EX	240-405	(5.42±1.20)(10)	0	0	2
75 MAR/KAU1 ¹⁾	EX	270-470	(5.36±0.78)(10)	0	0	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 SMI/ZEL ¹⁾ ¹⁾ k _a .	EX	240-406	(4.82±1.20)(10)	0	0	2
75 ZEL k _a . Flash-photolysis. Resonance-absorption.	EX	240-300	(4.8±1.2)(10)	0	0	2
81 NEL/MAR k _a . M = Ar. Flash-photolysis. Resonance-fluorescence at P(Total) = (10-50) torr. Laser-absorption at P(Total) = 10 torr.	EX	295	(4.94±1.08)(10)			2
82 MAR/JOH ²⁾ n = 0 assumed.	EX	218-363	(9.15±2.59)(9)	0	-644±79	2
82 MAR/JOH ²⁾ The preexponential factor expressed as: A(T/298) ^{-2.29} .	EX	218-363	(8.14±0.30)(10)	-2.29	0	2
²⁾ k _a . Flash-photolysis. Resonance-fluorescence. OH generated by Flash-photolysis of HONO ₂ . P(Ar) = (10-50) torr. P-independent k.						
82 MAR/WAT ³⁾	EX	228	1.84(11)			2
82 MAR/WAT ³⁾	EX	246	1.26(11)			2
82 MAR/WAT ³⁾	EX	298	7.17(10)			2
82 MAR/WAT ³⁾	EX	415	4.76(10)			2
³⁾ k _a . M = He. Flash-photolysis. Resonance-fluorescence. OH generated by reacting H with NO ₂ . P = 40 torr. [HONO ₂] = (0.6-8.0)×10 ¹⁵ molec.cm ⁻³ . Other k's, for the same temperatures as above, but at different pressures in the (0-300) torr. range, are also given. The P-dependence is weaker above 298 K, but stronger below 298 K. The addition complex of channel (c) is considered by the authors as the precursor of channel (a).						
81 WIN/RAV k _a + k _b . HONO ₂ /Ar (or SF ₆) flash-photolysis. Resonance-fluorescence. P = (13-60) torr.	EX	224-366	(9.15±2.29)(9)	0	-649±69	2
82 JOU/POU k _a + k _b . Discharge-flow-EPR. OH produced by reacting H with NO ₂ in excess. At 298 K only channel (a) occurs. P = (0.6-2.3) torr. [OH] ₀ = (0.1-7.0)×10 ¹⁰ molec.cm ⁻³ .	EX	251-403	(4.40±1.20)(9)	0	-876±85	2
82 KUR/COR k _a + k _b . Flash-photolysis of HONO ₂ . [HONO ₂] = (10-221) torr.	EX	225-296	(6.32±2.41)(9)	0	-759±100	2
82 RAV/EIS ⁴⁾ k _a + k _b . M = N ₂ . P(N ₂) = 50 torr.	EX	251	(1.17±0.14)(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 RAV/EIS ⁴) k _a + k _b . M = SF ₆ . P(SF ₆) = 60 torr.	EX	251	(1.26±0.10)(11)			2	
82 RAV/EIS ⁴) k _a + k _b . M = Ar. P(Ar) = 50 torr.	EX	298	(7.53±0.78)(10)			2	
82 RAV/EIS ⁴) k _a + k _b . M = SF ₆ . P(SF ₆) = 60 torr.	EX	298	(8.37±1.69)(10)			2	
82 RAV/EIS ⁴) k _a + k _b . M = SF ₆ .	EX	220-380	(9.15±2.29)(9)	0	-649±69	2	
⁴) Pulsed Laser-photolysis of HONO ₂ in Ar, N ₂ , or SF ₆ . Channel (a) is the major pathway.							
OH + HO ₂ NO ₂ → H ₂ O + O ₂ + NO ₂ (a) → H ₂ O ₂ + NO ₃ (b) → HO ₂ + HONO ₂ (c)							
Hydroxyl + Peroxynitric acid							
80 LIT k _a . Infrared Absorption Spectroscopy.	EX	263-283	(1.75±0.60)(12)	0	0	2	
82 BAR/BAS k _a . Reaction of OH with HO ₂ NO ₂ in a glass-cylinder. FTIR Spectroscopy. OH produced by the reaction: HO ₂ + NO ₂ → OH + NO ₃ . Supersedes 81 BAR/BAS.	EX	295	(2.47±0.60)(12)			2	
82 TRE/BLA ¹) k _a + k _b + k _c .	EX	246-324	(4.84±3.43)(12)	0	193±194	2	
82 TRE/BLA ¹) k _a + k _b + k _c . B = 0 assumed. (Recommended k.)	EX	246-324	(2.41±0.96)(12)	0	0	2	
¹) OH generated by reacting O(¹ D) with either H ₂ , or or H ₂ O. O(¹ D) obtained by Flash-photolysis of O ₃ .							
OH + CO → H + CO ₂ (a) → any other products (b)							
Hydroxyl + Carbon monoxide							
71 BRA/BEL1 k _a . M = Ar.	EX	1300-1900	4.2(11)	0	503±101	2	1.95
71 IZO/KIS k _a . Shock waves. Best data-fit. Total conc. = 5x10 ¹⁷ molec.cm ⁻³ .	DE	1400-2200	9.03(11)	0	503	2	
72 DIX ¹)	ES	1050	(2.4±0.12)(11)			2	
72 DIX ¹) Combination of present and other data.	SE	298-1330	3.09(11)	0	370±100	2	1.41
¹) k _a . Fuel-rich H ₂ /N ₂ /O ₂ flames.							
72 STU/NIK1 k _a . M = He (20 Torr).	EX	298	8.13(10)			2	1.15

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
73 DAY/THO k _a . Fuel-rich H ₂ /N ₂ /O ₂ flame k.	ES	1050	(2.4±0.12)(11)			2	
73 GAR/MAL k _a . M = Ar. Data-fit to a proposed mechanism.	EX	1200-2500	4.0(12)	0	4026	2	1.25
73 PEE/MAH1 k _a . Lean CH ₄ /O ₂ flames.	ES	1750	2.8(11)			2	
73 PEE/MAH1 k _a . Lean CH ₄ /O ₂ flames.	ES	1600-1900	1.36(12)	0	2768±101	2	
73 SMI/ZEL1 k _a . Within the 210-460 K range, slight positive T-dependence, possibly curved.	EX	300	8.7(10)			2	
73 WES/DEH1 k _a . Nonlinear Arrhenius behaviour. From 298 to 915 K, k increases from 8x10 ¹⁰ to 13.1x10 ¹⁰ cm ³ mol ⁻¹ s ⁻¹ .	EX	298	8.0(10)			2	
74 DAV/FIS k _a . M = He.	EX	220-373	(1.29±0.11)(11)	0	81±40	2	
74 HOW/EVE k _a . M = He, Ar, or N ₂ .	EX	296	9.40(10)			2	
74 TRA/ROS2 k _a . M = Ar. CO ₂ is vibrationally excited.	EX	300	7.53(10)			2	
75 BIO/LAZ k _a . Uninhibited CH ₄ /O ₂ /Ar flame.	EX	1250-1750	4.7(11)	0	0	2	
75 CAM/HAN1 k _a /k _{ref} . Estimated ratio. k _{ref} : OH + NO ₂ (+ M) → HNO ₃ (+ M).	RL	292	(5.3±1.0)(-2)			2/2	
75 GOR/MUL1 k _a . M=Ar (710 torr.) + H ₂ O (10 torr.) + CO (10 torr.)	EX	298	(9.07±0.05)(10)			2	
75 STE/ZEL k _a . Nonlinear Arrhenius behaviour. For 300-900 K: log k = (10.85±0.08 + 4.0x10 ⁻⁴ T (cm ³ mol ⁻¹ s ⁻¹ .)	EX	300	9.33(10)			2	1.20
75 TRA/ROS k _a . M = Ar. CO ₂ is vibrationally excited.	EX	300	7.53(10)			2	
75 VAN/PEE k _a . Lean CO/H ₂ /O ₂ flame. Non-linear Arrhenius behaviour. k increases slightly from 400 to 800 K.	EX	400	8.0(10)			2	
75 VAN/PEE k _a . Lean CO/OH ₂ /O ₂ flame. log k = (10.85±0.08) + 4.0x10 ⁻⁴ T cm ³ mol ⁻¹ s ⁻¹ .	EX	1000-1800	2.32(12)	0	2869	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 ZEL k _a . Flash -photolysis. Resonance-absorption. 2) k = 6.76x10 ¹⁰ exp(8.7x10 ⁻⁴ T) cm ³ mol ⁻¹ s ⁻¹ . (Empirical expression).	EX	220-900	2)	2)	2)	2 2.0
76 ATK/PER2 k _a . M = Ar. P = (25-634) torr. Limiting high-pressure k.	EX	299	(9.28±0.96)(10)			2
76 BRA/CAP k _a /k _{ref} . k _{ref} : OH + CH ₄ → H ₂ O + CH ₃	RL	1300	1.8(-1)			2/2
76 COX/DER1 k _a /k _{ref} . k _{ref} : OH + H ₂ → H ₂ O + H.	RL	298	(3.86±0.34)(1)			2/2
76 COX/DER1 k _a .	ES	298	(1.63±0.12)(11)			2
76 SIE/SIM1 k _a /k _{ref} . k _{ref} : OH + H ₂ → H ₂ O + H. Limiting high-pressure ratio.	RL	217-298	2.0(-1)	0	-1711	2/2
76 SIE/SIM1 k _a /k _{ref} . k _{ref} : OH + H ₂ → H ₂ O + H. Rate ratio increasing from a limiting low-pressure value of 14 to a limiting high-pressure value of 50.	RL	298	1.4(1)			2/2
77 ATR/BAL ³⁾ k _a /k _{ref} . k _{ref} : OH + H ₂ → H ₂ O + H.	RL	773	(2.35±0.20)(-1)			2/2
77 ATR/BAL ³⁾ k _a . 3) Aged boric-acid coated vessel. P(Total) = 500 torr.	RN	773	9.6(10)			2
77 CHA/USE ⁴⁾ k _a /k _{ref} . P = 100 torr.	RL	298	(5.86±0.84)(-2)			2/2
77 CHA/USE ⁴⁾ k _a . P = 100 torr.	RN	298	(8.28±1.18)(10)			2
77 CHA/USE ⁴⁾ k _a /k _{ref} . P = 700 torr.	RL	298	(1.27±0.07)(-1)			2/2
77 CHA/USE ⁴⁾ k _a . P = 700 torr.	RN	298	(1.79±0.98)(10)			2
4) k _{ref} : OH + (CH ₃) ₃ CH → H ₂ O + (CH ₃) ₃ C (a) → H ₂ O + (CH ₃) ₂ CHCH ₂ (b)						
77 OVE/PAR1 ⁵⁾ k _a . M = He. P = 50 torr.	EX	296	(1.22±0.05)(11)			2
77 OVE/PAR1 ⁵⁾ k _a . M = SF ₆ . P = (200-350) torr. 5) Limiting high-pressure k.	EX	296	(1.95±0.12)(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
78 BIE/ZET2 ⁶⁾ k _a . P(He, or N ₂) < 50 torr.	EX	297	9.03(10)			2
78 BIE/ZET2 ⁶⁾ k _a . P(He) = 740 torr.	EX	297	(1.20±0.22)(11)			2
78 BIE/ZET2 ⁶⁾ k _a . P(N ₂) = 740 torr.	EX	297	(1.38±0.20)(11)			2
78 BIE/ZET2 ⁶⁾ k _a . P(N ₂) = 745 torr.	EX	297	(1.70±0.17)(11)			2
78 BIE/ZET2 ⁶⁾ k _a . P(N ₂) = 750 torr.	EX	297	(8.67±1.26)(10)			2
⁶⁾ k dependent on pressure and purity-degree of M. UV-Photolysis. Resonance-absorption.						
78 BUT/SOL k _a . Quartz reactor. H ₂ O ₂ photolysis. Gas-chromatography. P(O ₂ + N ₂) = (100-600) torr.	EX	305	(1.62±0.24)(11)			2
79 CLY/HOL k _a . Resonance-fluorescence. Gas-chromatography.	EX	293-430	1.32(11)	0	88±40	2 1.3
79 ZEL k _a . ⁷⁾ k = exp(24.98+9.2x10 ⁻⁴ T) cm ³ mol ⁻¹ s ⁻¹ . Non-Arrhenius best-fit of all data. Critical evaluation.	EX	300-2000	⁷⁾	⁷⁾	⁷⁾	2
77 PER/ATK2 ⁹⁾ k _{overall} .	EX	299	⁸⁾			2
⁸⁾ k dependent on the nature and pressure of the third body. For M = Ar: k = (9.03±0.90)x10 ¹⁰ cm ³ mol ⁻¹ s ⁻¹ at 25.5 torr. increasing to k = (9.76±1.45)x10 ¹⁰ cm ³ mol ⁻¹ s ⁻¹ at 643.3 torr. For M = SF ₆ : k = (9.22±0.96)x10 ¹⁰ cm ³ mol ⁻¹ s ⁻¹ at 25.3 torr. increasing to k = (2.07±0.21)x10 ¹¹ cm ³ mol ⁻¹ s ⁻¹ at 603.5 torr. The assumed mechanism (73 SMI/ZEL) is: OH + CO → HOCO [†] (a) HOCO [†] → OH + CO (-a) HOCO [†] → H + CO ₂ (b) HOCO [†] + M → HOCO + M (c) (with HOCO [†] removed by O ₂) Steady-state treatment gives: k = k _a (k _b + k _c [M])/(k _a + k _b + k _c [M])						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
From this expression and the experimental data, estimates of individual rate constants and ratios obtained are: $k_a = 3.61 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$; $k_{-a} \sim 8 \times 10^9 \text{ s}^{-1}$; $k_b \sim 3 \times 10^9 \text{ s}^{-1}$; $k_c \sim 2.41 \times 10^{14} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$; $k_b / (k_{-a} + k_b) = 0.25$; $k_c / (k_{-a} + k_b) = 2.41 \times 10^4 \text{ cm}^3 \text{ mol}^{-1}$. ⁹) Flash-photolysis of H₂O vapor. Resonance-Fluorescence. P(Total) = (25-643) torr. M = Ar, or SF₆.						
OH + CO[†] → H + CO₂ Hydroxyl + Carbon monoxide						
81 DRE/WOL ¹)	EX	298	(9.1±3.4)(10)			2
T _t = T _r = T _v = 298K.						
81 DRE/WOL ¹)	EX	298	(8.2±3.0)(10)			2
T _t = T _r = 298K. T _v = 1400K.						
81 DRE/WOL ¹)	EX	298	(7.8±2.9)(10)			2
T _t = T _r = 298K. T _v = 1800K.						
¹) Discharge-flow.						
IR-resonance radiation.						
OD + CO → products ¹) Hydroxyl-d + Carbon monoxide						
82 PAR/IRW ²)	EX	298	(3.12±0.30)(10)			2
M = He. P(He) = 20 torr.						
82 PAR/IRW ²)	EX	298	(1.03±0.15)(11)			2
M = N ₂ . P(N ₂) = 650 torr.						
82 PAR/IRW ²)	EX	298	(1.07±0.07)(11)			2
M = CF ₄ , or SF ₆ . P(CF ₄ , or SF ₆) = 600 torr.						
¹) The assumed mechanism (73 SMI/ZEL) is:						
OD + CO → DOCO [†] (a)						
DOCO [†] → OD + CO (-a)						
DOCO [†] → D + CO ₂ (b)						
DOCO [†] + M → DOCO + M (c)						
(with DOCO [†] removed by O ₂ , or a radical)						
Steady-state treatment gives:						
k = k _a (k _b + k _c [M]) / (k _{-a} + k _b + k _c [M]). From						
this expression and the experimental data, indi-						
vidual rate constants and ratios obtained are:						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$k_a = (1.37 \pm 0.16) \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. M = CF ₄ , or N ₂ . Average k. $k_{-a} \approx 8.4 \times 10^8 \text{ s}^{-1}$. (Estimated k) $k_b \approx 1.9 \times 10^8 \text{ s}^{-1}$. (Estimated k) $k_{-a}/k_b = (4.4 \pm 0.7)$ M = CF ₄ , or N ₂ . Average ratio. $k_c/k_b = (4.3 \pm 1.4) \times 10^5$, for M = CF ₄ = (4.7 ± 1.4) × 10 ⁵ , for M = N ₂ = (1.4 ± 0.6) × 10 ⁵ , for M = He.						
2) Flash-photolysis of D ₂ O vapor in Vacuum-UV. Time-resolved Resonance-Absorption. [CO] = 3.0 × 10 ¹¹ molec.cm ⁻³ . P = (20-650) torr. Supersedes 81 PAR/IRW.						
OH(v=1) + CO → H + CO ₂						
Hydroxyl + Carbon monoxide						
77 SPE/END	EX	295	≤ 1.81(11)			2
77 SPE/GLA	EX	295	< 3.01(12)			2
OH(v=9) + CO ₂ → products						
Hydroxyl + Carbon dioxide						
72 WOR/COL	EX	298	(1.45 ± 0.60)(10)			2
OH + CH ₃ → H + H + HCHO (a)						
OH + CH ₃ → CH ₃ OH (b)						
Hydroxyl + Methyl						
80 BHA/FRA	EX	1700-2300	2.0(16)	0	13860	2
k_a . Shock-tube. Resonance-Absorption.						
81 TSU/KAT ¹⁾	RN	1500-1900	8.32(9)	0	9863	2
Total conc. = 6.0 × 10 ¹⁸ molec.cm ⁻³ .						
81 TSU/KAT ¹⁾	RN	1500-1900	4.90(10)	0	9382	2
Total conc. = 3.0 × 10 ¹⁹ molec.cm ⁻³ .						
81 TSU/KAT ¹⁾	DE	1500-1900	1.20(11)	0	8781	2
Total conc. = 6.0 × 10 ¹⁹ molec.cm ⁻³ .						
¹⁾ k_b . M = Ar. CH ₃ OH/O ₂ thermal oxidation behind reflected shock-waves. $k_1 = k_{-1}K$. Same data given in 81 TSU/HAS.						
80 SWO/HOC	EX	296	(5.6 ± 1.5)(13)			2
k_{overall} .						
Flash-photolysis of H ₂ O vapor.						
P ~ 760 torr.						
M = N ₂ , H ₂ .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH₄ → H₂O + CH₃						
Hydroxyl + Methane						
71 BAK/BAL Rate constant per CH bond.	CO	298-753	6.3(12)	0	2516	2
73 PEE/MAH1	EX	1100-1900	3.0(13)	0	3020	2
74 DAV/FIS	EX	240-373	(1.42±0.13)(12)	0	1711±88	2
74 MAR/KAU	EX	290-440	(2.31±0.12)(12)	0	1842±20	2
75 GOR/MUL1 ¹⁾	EX	381	(1.57±0.16)(10)			2
75 GOR/MUL1 ¹⁾	EX	416	(3.3±0.1)(10)			2
¹⁾ In an atmosphere of H ₂ O vapor.						
75 OVE/PAR	EX	295	(3.92±0.16)(9)			2
75 STE/ZEL	EX	300-700	2.8(12)	0	1862	2
76 COX/DER1 k _{ref} : OH + H ₂ → H ₂ O + H.	RL	298	(1.04±0.12)			2/2
76 COX/DER1	ES	298	(4.58±0.12)(9)			2
76 HOW/EVE1	EX	296	(5.72±0.84)(9)			2
76 ZEL/STE Flash-photolysis. Resonance-absorption. The exponential factor expressed as: A(T/298) ^{3.08} . Same data given in 75 ZEL.	EX	300-900	1.45(11)	3.08	1010	2 1.15
78 ERN/WAG ²⁾	EX	1300	(2.5±0.8)(12)			2
78 ERN/WAG ²⁾ Empirical fit. The preexponential factor expressed as: A(T/298) ^{2.13} .	EX	250-2000	2.89(11)	2.13	1234	2
²⁾ Flash-photolysis-Shock-tube technique.						
78 SHA The preexponential factor expressed as: A(T/298) ² .	CO	300-2500	7.56(11)	2.0	1485	2
79 ZEL Critical evaluation. The preexponential factor expressed as: A(T/298) ^{2.13}	SE	300-2000	2.89(11)	2.13	1233	2
80 SWO/HOC Flash-photolysis of H ₂ O vapor. P ~ 760 torr.	EX	296	(4.2±0.4)(9)			2
80 TUL/RAV ³⁾ Best-fit non-linear Arrhenius expression. The preexponential factor expressed as: A(T/298) ^{1.92} .	EX	298-1020	4.48(11)	1.92	1355	2
80 TUL/RAV ³⁾ ³⁾ M = Ar. Flash-photolysis. Resonance-fluorescence. P(H ₂ O) = 150 mtorr. P(CH ₄) = 0-1 torr. P(Ar) = 50 torr.	EX	298	(4.52±0.36)(9)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
82 FAI/SMI ⁴⁾	EX	830	(7.53±2.71)(11)			2	
82 FAI/SMI ⁴⁾	EX	1030	(7.82±2.41)(11)			2	
82 FAI/SMI ⁴⁾	EX	1400	(2.59±0.60)(12)			2	
⁴⁾ Two-laser method for real-time measurement of radical-molecule k's. OH generated by irradiation of a SF ₆ /N ₂ /H ₂ O ₂ /H ₂ O mixture at 40 torr., by a pulsed IR CO ₂ laser.							
82 JEO/KAU1 ⁵⁾	EX	269-473	(3.37±0.90)(12)	0	1973±101	2	
82 JEO/KAU1 ⁵⁾	EX	269-473	3.36(11)	2.0	1263	2	
Modified, non-linear Arrhenius expression. Optimized. The preexponential factor expressed as: A(T/298) ² .							
⁵⁾ Discharge-flow. Resonance-fluorescence. [CH ₄] = (0.23-8.85)×10 ¹⁵ molec.cm ⁻³ .							
OH(v=n) + CH ₄ → H ₂ O + CH ₃ Hydroxyl + Methane							
72 WOR/COL	EX	298	(8.43±1.20)(9)			2	
Unreported T assumed to be 298K.							
77 SPE/END	EX	295	≤1.81(10)			2	
Upper-limit k.							
OH + CDH ₃ → H ₂ O + CDH ₂ (a) → HDO + CH ₃ (b) Hydroxyl + Methane-d							
75 GOR/MUL1	EX	416	(2.2±0.1)(10)			2	
k _a + k _b . In an atmosphere of water vapor.							
OH + CD ₂ H ₂ → H ₂ O + CD ₂ H (a) → HDO + CDH ₂ (b) Hydroxyl + Methane-d ₂							
75 GOR/MUL1	EX	416	(1.8±0.1)(10)			2	
k _a + k _b . In an atmosphere of water vapor.							
OH + CD ₃ H → H ₂ O + CD ₃ (a) → DHO + CD ₂ H (b) Hydroxyl + Methane-d ₃							
75 GOR/MUL1	EX	416	(6.7±0.3)(9)			2	
k _a + k _b . In an atmosphere of water vapor.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
OH + CD₄ → DHO + CD₃							
Hydroxyl + Methane-d₄							
75 GOR/MUL1 In an atmosphere of H ₂ O vapor.	EX	416	(3.0±1.0)(9)			2	
OH + HCHO → H₂O + CHO (a)							
→ H ₂ O + CHO [†] (b)							
→ HCOOH + H (c)							
Hydroxyl + Formaldehyde							
71 MOR/NIK1 k _a .	EX	298	8.43(12)			2	1.25
71 MOR/NIK2 k _a .	EX	300	9.0(-1)			2/2	
k _{ref} : OH + CH ₃ CH=CH ₂ → products.							
73 PEE/MAH1 k _a .	ES	1400-1800	≈2.3(13)	0	0	2	
77 VAN/VAN k _a .	ES	300-1600	3.9(13)	0	705	2	
78 NIK/MAK ¹⁾ k _a /k _{ref} .	RL	298	(1.5±0.1)			2/2	
k _{ref} : OH + CH ₂ =CH ₂ → products.							
78 NIK/MAK ¹⁾ k _a .	RN	298	9.03(12)			2	
¹⁾ HCHO + HONO photolysis. FTIR-spectroscopy.							
78 ATK/PIT3 k _a . Flash-photolysis. Resonance-fluorescence.	EX	299-426	7.53(12)	0	88±151	2	
80 STI/NAV k _a + k _c . Flash-photolysis. Resonance-fluorescence. T-, and P-flash-intensity independent.	EX	228-362	(6.32±0.66)(12)	0	0	2	
78 HOR/SU k _b /k _c . HCHO photolysis at 313 nm. P(HCHO) = 8 torr. P(O ₂) = (0.02-8) torr. P(CO ₂) = (0-300) torr.	RL	298	≈5.0(-1)			2/2	
80 MOR/HEI k _b /(k _a + k _b + k _c). NO ₂ Photolysis at 366 nm., in presence of HCHO. IR absorption spectroscopy. k _{ref} : OH + HCHO → products.	RL	296	(4.9±1.6)(-1)			2/2	
78 SMI k _{overall} . Discharge-flow. Mass-spectrometry. k shows no significant trends when the [HCHO] and [OH] are varied by factors of 8 and 4, respectively, at 298 and 334 K. E _a = 1434±478 cal.mol ⁻¹ between 268 and 334 K.	RN	298	(3.91±0.90)(12)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + HCOOH → products						
Hydroxyl + Formic acid						
82 ZET/STU Pulsed Vacuum UV-photolysis of H ₂ O, Ar and HCOOH mixtures. Resonance-fluorescence. P(H ₂ O) = (0.03-0.2) torr. P(Ar) = (25-100) torr.	EX	298	(1.93±0.12)(11)			2
OH + CH₃OH → H₂O + CH₂OH (a) → H₂O + CH₃O (b)						
Hydroxyl + Methanol						
75 OSI/SIM (k _a + k _b)/k _{ref} . k _{ref} : OH + CO → H + CO ₂	RL	298	(6.3±1.0)(-1)			2/2
75 OSI/SIM (k _a + k _b)/k _{ref} . k _{ref} : OH + CO → H + CO ₂	RL	345	(9.8±2.0)(-1)			2/2
76 CAM/MCL k _a + k _b .	EX	292	(5.7±0.6)(11)			2
75 BOW2 k _a . M = Ar. Reflected shock waves. Best data-fit. [Ar] = (5.7-17.0)×10 ¹⁸ molec.cm ⁻³ . [CH ₃ OH] = 1.3×10 ¹⁷ molec.cm ⁻³ . [O ₂] = 2.5×10 ¹⁷ molec.cm ⁻³ .	ES	1545-2180	3.0(13)	0	3000	2
78 OVE/PAR1 k _a . Flash-photolysis. Resonance-aasorption.	EX	296	(6.4±0.6)(11)			2
78 RAV/DAV k _a + k _b . Flash-photolysis. Resonance- fluorescence. P(CH ₃ OH) = 10 torr.	EX	298	(6.02±0.60)(11)			2
81 TSU/HAS k _a . M = Ar, CH ₃ OH/O ₂ thermal oxidation in Ar, behind reflected shock-waves.	ES	1200-1800	2.0(14)	0	3007	2
81 VAN/VAN k _a . CH ₃ OH/O ₂ burned at 40 torr., with or without added Ar or H ₂ . Molecular beam-sampling.	DE	1000-2000	4.8(13)	0	2265	2
OH + CS₂ → SH + COS (a) → SOH + CS (b)						
Hydroxyl + Carbon disulfide						
80 COX/SHE ¹⁾ k _a /k _{ref} . k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	297	(6.0±2.0)(-2)			2/2
80 COX/SHE ¹⁾ k _a .	RN	297	(2.59±0.96)(11)			2
¹⁾ Photolysis of HONO and CS ₂ . Gas-chromatography. P = 760 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 IYE/ROW k _a . Photolysis of H ₂ O ₂ + CS ₂ mixtures. Gas-chromatography. Upper-limit k.	EX	298	<1.81(9)			2
82 LEU/SMI2 ²) k _a .	EX	298	≤4.22(9)			2
82 LEU/SMI2 ²) k _a . ²) Discharge-flow Resonance-fluorescence. OH generated by reacting H with NO ₂ . Upper-limit k's. P-independent in the (2.2-58) torr. range. [CS ₂] ₀ = (0.4-35.1) × 10 ¹⁵ molec.cm ⁻³ . [OH] ₀ = (0.7-3.7) × 10 ¹¹ molec.cm ⁻³ .	EX	520	≤1.81(9)			2
78 ATK/PER1 k _a + k _b . Upper-limit k.	EX	300-425	<4.22(10)			2
78 KUR2 k _a + k _b . Flash-photolysis. Resonance-fluorescence. Channel (a) is more probable than (b).	EX	296	(1.11±0.20)(11)			2
80 WIN/SHA ³) k _a + k _b .	EX	251	<5.96(9)			2
80 WIN/SHA ³) k _a + k _b .	EX	297	<9.03(8)			2
80 WIN/SHA ³) k _a + k _b . ³) Flash-photolysis. Resonance-fluorescence. M = Ar, or SF ₆ . Upper-limit k's. P(H ₂ O) = (230-250) mtorr. P = (35-50) torr.	EX	363	<9.64(8)			2
82 BIE/HAR k _a + k _b . Discharge-flow. OH generated by reacting H with NO ₂ . Upper-limit k. [OH] ₀ = (0.2-2.0) × 10 ¹² molec.cm ⁻³ . P (Total) ~ 2 torr. (He)	EX	298	≤3.01(10)			2
82 JON/BUR k _a /k _b . CS ₂ /HONO photolysis in N ₂ (or N ₂ /O ₂). COS is the principal product. P(O ₂) = (40-380) torr.	EX	295	(1.02±0.54)(12)			2
OH + COS → SH + CO ₂ (a) → SOH + CO (b)						
Hydroxyl + Carbon oxide sulfide						
80 COX/SHE ¹) k _a /k _{ref} . Upper-limit ratio. k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	297	≤5.0(-3)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 COX/SHE ¹⁾ k _a . Upper-limit k. ¹⁾ Photolysis of HONO and COS. Gas-chromatography. P(O ₂) = (40-380) torr. P = 760 torr.	RN	297	≤2.41(10)			2
78 ATK/PER1 k _a + k _b . Upper-limit k.	EX	299-430	<4.22(9)			2
78 KUR2 k _a + k _b . Flash-photolysis. Resonance-fluorescence.	EX	296	(3.41±0.73)(10)			2
80 RAV/KRE k _a + k _b . Laser-photolysis of Nitric acid. Flas-photolysis. Resonance-fluorescence. Upper-limit k.	EX	298	≤5.30(9)			2
81 LEU/SMI k _a + k _b . Discharge-flow. Resonance-fluorescence.	EX	300-520	(7.83±1.81)(11)	0	2300±100	2
OH(v=9) + COS → products Hydroxyl + Carbon oxide sulfide						
72 WOR/COL	EX	298	(1.51±0.90)(10)			2
OH + CH ₃ SH → products Hydroxyl + Methanethiol (Methylmercaptan)						
77 ATK/PER4 ¹⁾	EX	299-426	5.35(12)	0	-398±151	2
77 ATK/PER4 ¹⁾ ¹⁾ Flash-photolysis. Resonance-fluorescence.	EX	299-426	(2.04±0.20)(13)	0	0	2
80 COX/SHE ²⁾ k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	297	(1.13±0.11)(-1)			2/2
80 COX/SHE ²⁾ ²⁾ Photolysis of HONO and CH ₃ SH. Gas-chromatography. P = 760 torr.	RN	297	(5.44±0.51)(13)			2
81 WIN/KRE H ₂ O/Ar/CH ₃ SH flash-photolysis. Resonance-fluorescence. P(H ₂ O) = (0.05-0.15) torr. P(Ar) = (40-120) torr.	EX	244-367	(6.93±2.35)(12)	0	-338±100	2
OH + CN → H + NCO Hydroxyl + Cyanogen						
76 MOR Premixed flames. T-independent k. E _a = 0 assumed.	EX	2300-2560	6.03(13)	0	0	2
77 HAY2 Fuel-rich flames.	EX	1950-2380	(5.6±0.7)(13)	0	0	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
OH + HCN → H + HOCN (a)							
→ H ₂ O + CN (b)							
Hydroxyl + Hydrocyanic acid							
77 HAY2	EX	1950-2380	(2.0±0.2)(11)	0	0	2	
k _a . Fuel-rich flames.							
79 PHI2	EX	298-563	(3.23±0.65)(10)	-1.0	1860	2	
k _b . Discharge-flow. Resonance-fluorescence.							
The preexponential factor expressed as:							
A(T/298) ⁻¹ .							
P > 10 torr.							
OH + CH₃NH₂ → products							
Hydroxyl + Methanamine							
77 ATK/PER4 ¹)	EX	299-426	6.14(12)	0	-229±151	2	
77 ATK/PER4 ¹)	EX	298	(1.33±0.13)(12)			2	
¹) Flash-photolysis.							
Resonance-fluorescence.							
OH + NH₂NHCH₃ → products							
Hydroxyl + Hydrazine, methyl-							
79 HAR/ATK	EX	298-424	(3.91±0.79)(13)	0	0	2	
M = Ar. Flash-photolysis.							
Resonance-fluorescence.							
P(Ar) = (25-50) torr.							
OH + CH₃ONO → products							
Hydroxyl + Nitrous acid methyl ester (Methyl nitrite)							
75 CAM/GOO2	ES	292	(8.0±1.1)(11)			2	
82 AUD/BAU1	EX	295	(7.1±1.2)(11)			2	
Static system. OH generated by the chain reaction:							
H ₂ O ₂ + NO ₂ + CO.							
P < 75 torr. [CO] ₀ ~ 3.0x10 ¹⁸ molec.cm ⁻³ .							
[CH ₃ ONO] ₀ < 3.6x10 ¹⁷ molec.cm ⁻³ .							
[H ₂ O ₂] ₀ ~ 9.0x10 ¹⁵ molec.cm ⁻³ .							
[NO ₂] ₀ ~ 3.3x10 ¹⁶ molec.cm ⁻³ .							
OH + CH₃NO₂ → products							
Hydroxyl + Methane, nitro-							
75 CAM/GOO2	ES	292	(5.5±0.6)(11)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH ₂ =CH → H + CH ₂ =C=O (a)						
→ H ₂ + CH=C=O (b)						
→ CO + CH ₃ (c)						
→ H + CH=COH (d)						
→ [HO, CH=CH]* (e)						
Hydroxyl + Ethyne						
77 PER/ATK2	EX	288-422	1.15(12)	0	312±201	2
k _a (or, more likely, k _d .) M = Ar. P > 200 torr.						
77 VAN/VAN	ES	570-850	3.2(11)	0	101	2
k _a . M = O ₂ , or O ₂ + Ar.						
80 BAR/DOV	EX	2650	1.81(12)			2
k _a . Ethyne oxidation by water vapor behind shock-waves. Time-of-flight Mass-spectrometry. It is assumed that step (a) is followed by the fast dissociation of CH ₂ =C=O into CH ₂ and CO.						
82 BIT/HOW	EX	1700-1900	(1.3±0.3)(12)	0	0	2
k _a . C ₆ H ₆ /O ₂ /Ar flame. Molecular beam Mass-spectrometry. P = 20 torr.						
71 BRE/GLA	EX	295	(1.14±0.36)(11)			2
k _b . Channel (b) is preferable to the possible abstraction path: OH + CH ₂ =CH → H ₂ O + CH=C						
77 VAN/VAN	ES	650-1110	5.5(13)	0	6895	2
k _c . M = O ₂ , or O ₂ + Ar.						
81 TSU/KAT	ES	1500-1900	2.0(13)	0	1564	2
k _c . CH ₃ OH/O ₂ thermal oxidation in Ar, behind reflected shock-waves. UV-absorption. IR-emission. Same data given in 81 TSU/HAS.						
73 SMI/ZEL1	EX	210-460	1.2(12)	0	253	2
k _a + k _b + k _c . M = He.						
74 PAS/CAR1	EX	298	(1.20±0.36)(11)			2
k _a + k _b + k _c . M = He.						
75 DAV/FIS	EX	300	(9.94±0.90)(10)			2
k _a + k _b + k _c . M = He. Channel (a) gives probably the primary products. P-independent k.						
74 PAS/CAR2	EX	298	(1.76±0.16)(11)			2
k _a + k _b + k _c . Discharge-flow. P ~ 1 torr.						
77 DAV	EX	298	(9.94±0.90)(10)			2
k _a + k _b + k _c . Channel (a) is probably predominant. M = He. Flash-photolysis. Resonance-fluorescence. P(He) = (20-500) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
80 MIC/NAV ¹⁾ Low-pressure k. (Given with caution).	EX	228-413	≈2.41(11)	0	0	2	
80 MIC/NAV ¹⁾ High-pressure k.	EX	228-413	(4.11±0.72)(12)	0	646±47	2	
¹⁾ k _e . Channel (e) may be possibly followed by channel (a). Flash-photolysis. Resonance-fluorescence. P = (10-1100) torr.							
82 PER/WIL k _e . Channel (e) is followed by channel (a), or, possibly, (d). M = Ar. Resonance-fluorescence. OH generated by Vacuum-UV Photolysis of H ₂ O. Mass-spectrometry. P = (200-403) torr. (High-pressure k.) P-dependent for P < 200 torr. For the entire P-range of (0-403) torr. the following empirical expression holds: $k(T, P)_{bi} = [7.11 \times 10^{11} \exp(-165 \pm 200/T)] / [(30/P) + 1]$	EX	297-429	9.34(11)	0	244	2	
OH + CH ₂ =CH ₂ → CH ₂ CH ₂ OH → products (a) → H ₂ O + CH ₂ =CH (b)							
Hydroxyl + Ethene							
71 MOR/NIK2 k _a /k _{ref} . k _{ref} : CH ₃ CH=CH ₂ + OH → products.	RL	300	1.0(-1)			2/2	
71 MOR/STE k _a .	EX	300	1.08(12)			2	1.25
73 BRA/HAC k _a .	EX	298	(1.0±0.3)(12)			2	
73 SMI/ZEL1 k _a .	EX	210-460	4.5(12)	0	108	2	
73 STU1 k _a .	EX	298	(1.81±0.60)(12)			2	
74 STU1 k _a . UV Photolysis and Resonance-fluorescence.	EX	298	(1.81±0.60)(12)			2	
75 COX k _a . Rate constant expressed as αk with α ~3.0	RN	300	(5.66±0.60)(12)			2	
75 DAV/FIS ¹⁾ P = 3 torr.	EX	300	1.35(12)			2	1.3
75 DAV/FIS ¹⁾ P = 300 torr.	EX	300	3.21(12)			2	1.1
¹⁾ k _a . M = He. Pressure-dependent k.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 GOR/MUL1 k_a . In an atmosphere of water vapor.	EX	381	(3.75±0.20)(12)			2
75 GOR/MUL1 k_a . In an atmosphere of water vapor.	EX	416	(4.4±0.2)(12)			2
75 PAS/CAR Rate constant expressed as nk_a , where n is a stoichiometric factor.	EX	300	(1.39±0.08)(12)			2
76 HOW k_a . M = He. Limiting high-pressure k.	EX	296	2.41(12)			2
76 LLO/DAR2 k_a/k_{ref} . k_{ref} : OH + CH ₃ CH ₂ CH ₂ CH ₃ → products.	RL	305	2.88			2/2
76 LLO/DAR2 k_a .	RN	305	(5.2±1.0)(12)			2
77 ATK/PER2 ²⁾	EX	299-425	1.3(12)	0	-388±151	2
77 ATK/PER2 ²⁾	EX	299	(4.73±0.48)(12)			2
²⁾ k_a . M = Ar. Limiting high-pressure k.						
77 DAV ³⁾ M = N ₂ . P(N ₂) = 3 torr.	EX	298	(2.19±0.12)(12)			2
77 DAV ³⁾ M = He. P(He) = 3 torr.	EX	298	(1.35±0.13)(12)			2
77 DAV ³⁾ M = He. P(He) = 300 torr.	EX	298	(3.21±0.39)(12)			2
³⁾ k_a . Flash-photolysis. Resonance-fluorescence.						
77 OVE/PAR2 k_a . M = H ₂ O, SF ₆ , CF ₄ . Limiting high-pressure k.	EX	296	(6.0±1.0)(12)			2
78 OVE/PAR2 ⁴⁾ k_a . M = He. P(He) = 50 torr.	EX	298	(5.4±0.5)(12)			2
78 OVE/PAR2 ⁴⁾ k_a . M = SF ₆ , or CF ₄ . P(SF ₆ , or CF ₄) = 400 torr.	EX	298	(6.5±0.5)(12)			2
⁴⁾ Vacuum UV photolysis of H ₂ O.						
78 FRE k_a . Laser Magnetic Resonance Spectrometry.	EX	293	(4.7±1.5)(11)			2
80 COX k_a . HONO photosensitized oxidation in synthetic air. Gas-chromatography. [HONO] = (3-20) ppm. [NO] = NO ₂] = (0.3-3.0) ppm.	SE	300	4.82(12)			2
80 FAR/SMI k_a . M = He. Discharge flow. Resonance-fluorescence. Mass-spectrometry.	EX	298	(1.12±0.18)(19)			3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 ATK/ASC2 ⁵⁾	RL	299	(1.12±0.05)			2/2
$k_a k_{ref}$. k_{ref} : OH +  → products.						
82 ATK/ASC2 ⁵⁾	RN	299	(5.11±0.23)(12)			2
k_a . ⁵⁾ CH ₃ ONO/NO/CH ₂ =CH ₂ and Cyclohexane photolysis. [CH ₃ ONO] ₀ = (9.5-3.5)×10 ¹⁴ molec.cm ⁻³ . [CH ₂ =CH ₂] = (1.2-2.4)×10 ¹³ molec.cm ⁻³ . [NO] ₀ ~ 1.19×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.						
76 BRA/CAP	RL	1300	2.33			2/2
k_b/k_{ref} . k_{ref} : CH ₄ + OH → CH ₃ + H ₂ O						
76 MEA/HEI	RL	298	2.6(-1)			2/2
$k_b/(k_a + k_b)$.						
OH + CD ₂ =CD ₂ → products						
Hydroxyl + Ethene-d ₄						
78 NIK/MAK	RL	298	(1.03±0.06)			2
k_{ref} : OH + CH ₂ =CH ₂ → products. CD ₂ =CD ₂ /HONO Photolysis. FTIR-Spectroscopy. P(air) = 700 torr.						
OH + CH ₃ CH ₃ → H ₂ O + CH ₃ CH ₂						
Hydroxyl + Ethane						
71 BAK/BAL	CO	298-753	1.45(13)	0	1772	2
Rate constant per CH bond.						
71 BAK/BAL ¹⁾	RL	753	(1.05±0.11)(1)			2/2
79 BAL/WAL1 ¹⁾	RL	753-773	1.28	0	-1070	2/2
A and B recalculated from an empirical formula.						
¹⁾ k_{ref} : OH + H ₂ → H ₂ O + H.						
75 GOR/MUL1 ²⁾	EX	381	(4.0±0.2)(11)			2
75 GOR/MUL1 ²⁾	EX	416	(4.8±0.3)(11)			2
²⁾ In an atmosphere of water vapor.						
75 HUC/BOO ³⁾	RL	653	(9.6±1.1)			2/2
75 OVE/PAR	EX	295	(1.59±0.10)(11)			2
76 BRA/CAP ³⁾	RL	1300	2.88			2/2
³⁾ k_{ref} : OH + CH ₄ → H ₂ O + CH ₃						
76 HOW/EVE2	EX	296	(1.75±0.36)(11)			2
79 LEU	EX	298	(1.57±0.24)(11)			2
Discharge-flow. Resonance-fluorescence.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 LEE/TAN Discharge-flow. Resonance-fluorescence. OH generated by reacting H with NO ₂ .	EX	295	(1.39±0.24)(11)			2	
OH + CH ₂ =C=O → CHO + HCHO Hydroxyl + Ethenone (Ketene)							
77 VAN/VAN	ES	480-1000	2.8(13)	0	0	2	
OH + CH ₃ CHO → H ₂ O + CH ₃ CO (a) → H ₂ O + CH ₂ CHO (b) Hydroxyl + Acetaldehyde							
71 MOR/NIK2 k _a + k _b . k _{ref} : CH ₃ CH=CH ₂ + OH → products.	RL	300	9.0(-1)			2/2	
71 MOR/STE k _a + k _b . Channel (a) is predominant.	EX	300	9.03(12)			2	1.25
76 COX/DER3 k _a . Upper-limit k.	EX	296	≤1.2(13)			2	
78 ATK/PIT3 k _a + k _b . Flash-photolysis. Resonance-fluorescence.	EX	299-426	4.14(12)	0	257±151	2	
78 NIK/MAK ¹⁾ k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(1.9±0.2)			2/2	
78 NIK/MAK ¹⁾ ¹⁾ k _a + k _b . CH ₂ =CH ₂ /HONO photolysis. FTIR-spectroscopy. P(air) = 700 torr.	RN	298	9.64(12)			2	
81 KER/SHE ¹⁾ (k _a + k _b)/k _{ref} . k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(1.50±0.50)			2/2	
81 KER/SHE ¹⁾ k _a + k _b . ¹⁾ HONO/Synthetic air/Ethene/aldehyde photolysis.	RN	298	(7.23±2.41)(12)			2	
OH + CH ₃ COOH → products Hydroxyl + Acetic acid							
82 ZET/STU H ₂ O/Ar/CH ₃ COOH photolysis. Resonance-fluores- cence. P(Ar) = (20-500) torr. P(H ₂ O) = 0.1 torr.	EX	298	(3.61±0.72)(11)			2	
OH + CH ₃ CH ₂ OH → H ₂ O + CH ₃ CHOH (a) → any other products (b) Hydroxyl + Ethanol							
82 NAT/BHA k _a . M = O ₂ + Ar. Ethanol/O ₂ /Ar ignition behind reflected shock-waves. Data-fit. P = (1-2) atm.	ES	1300-1700	3.00(13)	0	3000	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 CAM/MCL k_{overall}	EX	292	(1.8±0.2)(12)			2
78 OVE/PAR1 k_{overall} . Flash-photolysis. Resonance-fluorescence.	EX	296	(2.25±0.22)(12)			2
78 RAV/DAV k_{overall} . Flash-photolysis. Resonance-fluorescence. P(Ethanol) < 2.5 torr.	EX	298	(1.58±0.22)(12)			2
OH + (CH₃)₂O → H₂O + CH₂OCH₃						
Hydroxyl + Methane, oxybis-						
77 PER/ATK1	EX	299-427	7.77(12)	0	388±151	2
77 PER/ATK1	EX	299	(2.11±0.21)(12)			2
OH + (CH₃)₂S → products						
Hydroxyl + Methane, thiobis-						
78 ATK/PER1 Flash-photolysis. Resonance-fluorescence.	EX	300-427	(3.29±0.72)(12)	0	-179±151	2
78 KUR1 Flash-photolysis. Resonance-fluorescence. Recommended k.	EX	273-426	(3.66±1.53)(12)	0	134±135	2
80 COX/SHE ¹⁾ k_{ref} : OH + CH ₂ =CH ₂ → products.	RL	297	(1.14±0.18)			2/2
80 COX/SHE ¹⁾ ¹⁾ Photolysis of HONO and (CH ₃) ₂ S. P = 760 torr.	RN	297	(5.48±0.84)(12)			2
81 WIN/KRE Flash-photolysis of H ₂ O/Ar/(CH ₃) ₂ S mixtures. P(H ₂ O) = (0.05-0.15) torr. P(Ar) = (50-200) torr.	EX	244-367	(4.10±0.66)(12)	0	138±46	2
OH + CH₃SSCH₃ → products						
Hydroxyl + Disulfide, dimethyl-						
80 COX/SHE ¹⁾ k_{ref} : OH + CH ₂ =CH ₂ → products.	RL	297	(2.8±1.0)(1)			2/2
80 COX/SHE ¹⁾ ¹⁾ Photolysis of HONO and CH ₃ SSCH ₃ . P = 760 torr.	RN	297	(1.34±0.48)(14)			2
81 WIN/KRE Flash-photolysis of H ₂ O/Ar/CH ₃ SSCH ₃ mixtures. P(Ar) = (50-200) torr. P(H ₂ O) = 0.06 torr.	EX	244-367	(3.55±1.99)(13)	0	-380±160	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{OH} + \text{NCCN} \rightarrow [\text{C}_2\text{N}_2\text{OH}]^\ddagger \text{ (a)}$ $\rightarrow \text{HOCN} + \text{CN} \text{ (b)}$						
Hydroxyl + Ethanedinitrile						
79 PHI1 k_a . Discharge-flow. Resonance-fluorescence. P = (1-16) torr.	EX	300-550	(1.87±0.28)(11)	0	1448	2
78 ATK/PER2 ¹⁾	EX	298	≤1.81(10)			2
78 ATK/PER2 ¹⁾	EX	424	≤3.01(10)			2
¹⁾ k_b . Flash-photolysis. Resonance-fluorescence. Upper-limit k's.						
$\text{OH} + \text{CH}_3\text{CN} \rightarrow \text{products}$						
Hydroxyl + Acetonitrile						
81 HAR/KLE OH produced by pulsed vacuum-UV photolysis of H_2O in a reaction vessel. Resonance-fluorescence.	EX	298-424	3.53(11)	0	755±126	2
$\text{OH} + \text{CH}_3\text{N}=\text{NCH}_3 \rightarrow \text{products}$						
Hydroxyl + Diazene, dimethyl- (Azomethane)						
79 KLA/AND Flash-photolysis. Resonance-fluorescence.	EX	368	(4.94±1.33)(11)			2
$\text{OH} + \text{CH}_3\text{CH}_2\text{NH}_2 \rightarrow \text{products}$						
Hydroxyl + Ethanamine						
78 ATK/PER3 Flash-photolysis. Resonance-fluorescence.	EX	298-426	8.85(12)	0	-189±151	2
$\text{OH} + (\text{CH}_3)_2\text{NH} \rightarrow \text{H}_2\text{O} + (\text{CH}_3)_2\text{N} \text{ (a)}$ $\rightarrow \text{H}_2\text{O} + \text{CH}_2\text{NHCH}_3 \text{ (b)}$						
Hydroxyl + Methanamine, N-methyl-						
79 LIN/CAL $k_a/(k_a + k_b)$. Long-path FTIR-Spectroscopy.	RL	298	(3.7±0.5)(-1)			2/2
78 ATK/PER3 $k_a + k_b$. Flash-photolysis. Resonance-fluorescence.	EX	298-426	1.7(13)	0	-247±150	2
$\text{OH} + \text{CH}_3\text{C}(\text{O})\text{O}_2\text{NO}_2 \rightarrow \text{products}$						
Hydroxyl + Peroxide, acetyl nitro-						
77 WIN/LLO Upper-limit k.	EX	299	≤1.0(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH₃CH₂ONO → products						
Hydroxyl + Nitrous acid ethyl ester (Ethyl nitrite)						
82 AUD/BAU1	EX	295	(1.15±0.23)(12)			2
Static system. OH generated by the reaction:						
$\text{H}_2\text{O}_2 + \text{NO}_2 + \text{CO}$						
P < 75 torr. [CO] ₀ ~ 3.0x10 ¹⁸ molec.cm ⁻³ .						
[CH ₃ CH ₂ ONO] ₀ < 3.6x10 ¹⁷ molec.cm ⁻³ .						
[H ₂ O ₂] ₀ ~ 9.0x10 ¹⁵ molec.cm ⁻³ .						
[NO ₂] ₀ ~ 3.3x10 ¹⁶ molec.cm ⁻³ .						
OH + O=C=C=O → CO₂ + CH=C=O						
Hydroxyl + 1,2-Propadiene-1,3-dione						
77 FAU/WAG2	EX	295-480	(7.0±3.0)(12)	0	620±160	2
OH + CH₃C≡CH → products						
Hydroxyl + 1-Propyne						
73 BRA/HAC	EX	298	(5.7±1.0)(11)			2
OH + CH₂=C=CH₂ → products						
Hydroxyl + 1,2-Propadiene						
73 BRA/HAC	EX	298	(2.7±1.5)(12)			2
77 ATK/PER3	EX	299-424	3.37(12)	0	-154±151	2
77 ATK/PER3	EX	299	(5.60±0.56)(12)			2
OH + CH₃CH=CH₂ → [CH₃CH=CH₂.OH] → products (a)						
→ H ₂ O + CH ₂ CH=CH ₂ (b)						
→ H + CH ₃ CH ₂ CHO (c)						
→ HCHO + CH ₃ CH ₂ (d)						
→ H + (CH ₃) ₂ CO (e)						
→ CH ₃ CHO + CH ₃ (f)						
Hydroxyl + 1-Propene						
71 MOR/NIK2	RL	300	1.0			2/2
k _a /k _{ref} . k _{ref} : OH + CH ₂ =CH ₂ → products.						
73 SIM/HEI2	RL	373-473	1.93(1)	0	-503	2/2
k _a /k _{ref} . k _{ref} : OH + CO → H + CO ₂ . Rate-ratio						
expression based on only two values: 75.0 at						
373 K and 55.0 at 473 K. The ratio of A-factors,						
19.3, is correction for an apparent misprint.						
74 GOR/VOL	RL	298	8.93(1)			2/2
k _a /k _{ref} . k _{ref} : OH + CO → CO ₂ + H.						
76 LLO/DAR2	RL	305	9.7			2/2
k _a /k _{ref} . k _{ref} : OH + CH ₃ CH ₂ CH ₂ CH ₂ → products.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
76 WIN/LLO k_a/k_{ref} . k_{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.	RL	305	4.9(-1)			2/2	
76 WU/JAP k_a/k_{ref} . Cylindrical Pyrex Reactor. k_{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products. P = 760 torr.	RL	303	4.0(-1)			2/2	
71 MOR/STE ¹⁾	EX	300	1.02(13)			2	1.25
73 SIM/HEI2 ¹⁾	RN	373-473	8.19(12)	0	50	2	
73 SIM/HEI2 ¹⁾ Extrapolated k.	ES	298	6.63(12)			2	
73 STU1 ¹⁾	EX	298	(8.73±1.33)(12)			2	
74 GOR/VOL ¹⁾	RN	298	(8.07±2.05)(12)			2	
75 ATK/PIT ¹⁾	EX	297-425	2.47(12)	0	-544±151	2	
75 ATK/PIT ¹⁾	EX	298	(1.5±0.15)(13)			2	
75 COX ¹⁾ Expressed as αk with $\alpha \sim 2.4$	RN	300	(2.17±0.24)(13)			2	
75 GOR/MUL1 ¹⁾ In an atmosphere of water vapor.	EX	381	(8.6±0.4)(12)			2	
75 GOR/MUL1 ¹⁾ In an atmosphere of water vapor.	EX	416	(1.2±0.06)(13)			2	
75 PAS/CAR ¹⁾ Expressed as nk (n = stoichiometric factor.)	EX	300	(3.01±0.60)(12)			2	
76 LLO/DAR2 ¹⁾	RN	305	(1.75±0.35)(13)			2	
76 WIN/LLO ¹⁾ ¹⁾ k_a .	RN	305	(1.49±3.0)			2	
78 NIP/PAR k_a . Flash-photolysis. Resonance-absorption.	EX	298	(1.47±0.08)(13)			2	
74 STU1 k_a . Pulsed vacuum UV Photolysis. Resonance-fluorescence.	EX	298	(8.73±1.32)(12)			2	
77 DAV ²⁾ k_a . M = He. P(He) = 20 torr.	EX	298	(1.54±0.07)(13)			2	
77 DAV ²⁾ k_a . M = He. P(He) = 200 torr.	EX	298	(1.58±0.07)(13)			2	
²⁾ Flash-photolysis. Resonance-fluorescence.							
78 OVE/PAR2 k_a . M = He, or SF ₆ . P-independent k. Vacuum-UV Photolysis of H ₂ O.	EX	298	(2.5±0.5)(13)			2	
78 PIT/ATK k_a . Irradiation of Propene-air mixtures in an all-glass chamber. P(Total) = 760 torr.	RN	298	(1.75±0.36)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
78 PIT/ATK k _a . Flash-photolysis. Resonance-fluorescence. P ~ (15-650) torr.	EX	298	(1.51±0.15)(13)			2
78 RAV/WAG ³) k _a . M = He. P(He) = 20 torr.	EX	298	(1.54±0.07)(13)			2
78 RAV/WAG ³) k _a . M = He. P(He) = 200 torr. ³) Flash-photolysis. Resonance-fluorescence.	EX	298	(1.58±0.07)(13)			2
79 NIP/PAR k _a . Flash-photolysis. Resonance-fluorescence.	EX	297	(1.48±0.17)(13)			2
82 ATK/ASC2 k _a . Mean of three previously reported k's.	SE	299	1.52(13)			2
73 BRA/HAC k _b .	EX	298	(3.0±1.0)(12)			2
73 GOR k _b . Lower-limit k.	EX	298	≥8.25(12)			2
80 COX/DER1 k _b . Photolysis of HONO + CH ₃ CH=CH ₂ at 760 torr. Gas-chromatography. Same data given in 80 COX.	RN	298	1.45(13)			2
82 BIE/HAR k _b /k _a .	RL	298	<2.0(-2)			2/2
79 HOY/SIE2 k _d /k _c . Low pressure nozzle reactor. Mass-spectrometry. P ~ (0.2-1.8) torr.	RL	298	(4.0±1.5)			2/2
79 HOY/SIE2 k _f /k _e . Low pressure nozzle. P ~ (0.2-1.8) torr.	RL	298	(3.5±1.5)			2/2
OH + CD ₃ CH=CH ₂ → products						
Hydroxyl + 1-Propene-3,3,3-d ₃						
73 STU1	EX	298	(8.73±1.33)(12)			2
OH + CH ₃ CD=CD ₂ → products						
Hydroxyl + 1-Propene-1,1,2-d ₃						
73 STU1	EX	298	(8.73±1.33)(12)			2
OH + CD ₃ CD=CD ₂ → products						
Hydroxyl + 1-Propene-d ₆						
71 MOR/NIK2 k _{ref} : OH + CH ₃ CH=CH ₂ → products.	RL	300	1.1			2/2
73 STU1	EX	298	(1.01±0.15)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{OH} + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{H}_2\text{O} + (\text{CH}_3)_2\text{CH} \quad (\text{a})$ $\rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}_2\text{CH}_2 \quad (\text{b})$						
Hydroxyl + Propane						
71 BAK/BAL k _a . Rate constant per secondary CH bond.	CO	298-753	2.2(13)	0	1283	2
71 BAK/BAL ¹⁾ k _a /k _{ref} . Estimated ratio per primary CH bond.	RL	753	5.25			2/2
78 DAR/ATK k _a . Irradiation technique. k computed from an empirical formula.	CO	300	6.99(11)			2
79 BAL/WAL1 ¹⁾ k _a /k _{ref} . A and B recalculated from an empirical formula.	RL	753-773	3.46(-1)	0	-1820	2/2
82 ATK/ASC3 k _a . Calculated from an empirical formula.	RN	299	5.06(11)			2
71 BAK/BAL ¹⁾ k _b /k _{ref} . Estimated ratio per secondary CH bond.	RL	753	1.1(1)			2/2
78 DAR/ATK k _b . Irradiation technique. k computed from an empirical formula.	CO	300	2.35(11)			2
79 BAL/WAL1 ¹⁾ k _b /k _{ref} . Calculated from an empirical formula.	RL	753-773	1.28	0	-1070	2/2
¹⁾ k _{ref} : $\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$.						
82 ATK/ASC3 k _b .	ES	299	1.14(11)			2
73 BRA/HAC ²⁾	EX	298	(5.0±1.0)(11)			2
73 GOR ²⁾	EX	298	(1.17±0.18)(12)			2
74 GOR/VOL ²⁾	RN	298	(1.33±0.36)(12)			2
75 GOR/MUL1 ²⁾ In an atmosphere of water vapor.	EX	381	(1.3±0.06)(12)			2
75 GOR/MUL1 ²⁾ In an atmosphere of water vapor.	EX	416	(1.15±0.05)(12)			2
75 HAR/BUR ²⁾	EX	329	(1.19±0.05)(12)			2
75 OVE/PAR ²⁾	EX	295	(1.22±0.06)(12)			2
78 DAR/ATK ²⁾ Irradiation technique.	EX	300	(9.58±1.33)(11)			2
80 COX/DER1 ²⁾ HONO photosensitized oxidation in syntnrhetic air. [HONO] = (3-20) ppm. [NO] = NO ₂ = (0.3-3.0) Same data given in 80 COX.	RN	300	1.14(12)			2
²⁾ k _a + k _b .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 ATK/ASC3 ³) $k_a + k_b$.	RN	299	(7.35±0.30)(11)			2
71 BAK/BAL ($k_a + k_b$)/ k_{ref} . k_{ref} : OH + H ₂ → H ₂ O + H.	RL	753	(2.15±0.22)(1)			2/2
74 GOR/VOL ($k_a + k_b$)/ k_{ref} . k_{ref} : OH + CO → CO ₂ + H.	RL	298	1.43(1)			2/2
75 HUC/BOO ($k_a + k_b$)/ k_{ref} . k_{ref} : OH + CH ₃ CH ₃ → H ₂ O + CH ₃ CH ₂	RL	653	(2.18±0.28)			2/2
82 ATK/ASC3 ³) ($k_a + k_b$)/ k_{ref} . k_{ref} : OH + CH ₃ CH ₂ CH ₂ CH ₃ → products.	RL	299	(4.73±0.16)(-1)			2
³) Photolysis of CH ₃ ONO/NO/Propane mixtures. P(Total) = 735 torr. [NO] ₀ = 1.2x10 ¹⁴ molec.cm ⁻³ . [Propane] = (1.2-2.4)x10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (2.1-4.0)x10 ¹⁴ molec.cm ⁻³ .						
OH + CH ₂ =CHCHO → H ₂ O + CH ₂ =CHCO (a) → any other products (b)						
Hydroxyl + 2-Propenal (Acrolein)						
80 MAL/CHI k_a . Photooxidation of 2-Propenal/Butane/Nitric oxide/Air mixtures in a smog chamber. k determined relative to the reaction: OH + CH ₃ CH ₂ CH ₂ CH ₃ → products.	RN	298	(1.6±0.2)(13)			2
81 KER/SHE ¹) $k_{overall}/k_{ref}$. k_{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(2.38±0.28)			2/2
81 KER/SHE ¹) $k_{overall}$.	RN	298	(1.14±0.12)(13)			2
¹) HONO/Synthetic air/Ethene/aldehyde photolysis.						
OH + CH ₃ C(O)CHO → products						
Hydroxyl + Propanal, 2-oxo- (Methylglyoxal)						
82 KLE/HAR OH generated by H ₂ O photolysis in Ar. Resonance-fluorescence. P(Total) = 50 torr.	EX	297	(4.28±0.96)(12)			2
OH + CH ₂ =CHCH ₂ OH → products						
Hydroxyl + 2-Propen-1-ol (Allyl alcohol)						
75 GOR/MUL1 In an atmosphere of water vapor.	EX	440	(1.56±0.2)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH₂=CHOCH₃ → products						
Hydroxyl + Ethene, methoxy-						
77 PER/ATK1	EX	299-427	3.67(12)	0	-511±151	2
77 PER/ATK1	EX	299	(2.02±0.20)(13)			2
OH + CH₃CH₂CHO → H₂O + CH₃CH₂CO (a)						
→ H₂O + CH₃CHCHO (b)						
→ H₂O + CH₂CH₂CHO (c)						
Hydroxyl + Propanal						
71 MOR/NIK2 (k _a + k _b + k _c)/k _{ref} . k _{ref} : OH + CH ₃ CH=CH ₂ → products.	RL	300	1.8			2/2
72 VOL/GOR k _a + k _b + k _c .	EX	298	(2.29±0.90)(12)			2
78 NIK/MAK ¹⁾ k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(2.6±0.1)			2
78 NIK/MAK ¹⁾ ¹⁾ k _a + k _b + k _c . CH ₃ CH ₂ CHO/HONO Photolysis. FTIR-Spectroscopy. P(air) = 700 torr.	RN	298	1.26(13)			2
81 AUD/BAU ²⁾ (k _a + k _b + k _c)/k _{ref} . k _{ref} : OH + CH ₃ CHO → products.	RL	298	(1.14±0.13)			2/2
81 AUD/BAU ²⁾ k _a + k _b + k _c .	RN	298	(1.08±0.14)(13)			2
²⁾ Linear, boric-acid-coated flow tube. Gas-chromatography. Channel (a) is predominant. P(Total) = 299 torr.						
81 KER/SHE ³⁾ (k _a + k _b + k _c)/k _{ref} . k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(2.28±0.17)			2/2
81 KER/SHE ³⁾ k _a + k _b + k _c .	RN	298	(1.08±0.06)(13)			2
³⁾ HONO/Synthetic air/Ethene/aldehyde photolysis.						
OH + (CH₃)₂CO → H₂O + CH₂C(O)CH₃						
Hydroxyl + 2-Propanone						
80 COX/DER1 HONO photosensitized oxidation in synthetic air. Gas-chromatography. Same data given in 80 COX. [NO] = NO ₂] = (0.3-3.0) ppm. [HONO] = (3-20) ppm.	RN	300	3.01(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH₃CH₂COOH → products						
Hydroxyl + Propanoic acid						
82 ZET/STU H ₂ O/Ar/Propanoic acid photolysis. Resonance-fluorescence. P(H ₂ O) = (0.02-0.22) torr. P(Ar) = 100 torr.	EX	298	(9.64±0.72)(11)			2
OH + CH₃C(O)OCH₃ → H₂O + CH₃C(O)OCH₂ (a) → H₂O + CH₂C(O)OCH₃ (b)						
Hydroxyl + Acetic acid methyl ester (Methyl acetate)						
78 CAM/PAR k _a + k _b . Reaction in a Pyrex vessel. Vacuum system. OH generated by reaction of a H ₂ O ₂ /NO ₂ /CO mixture. Channel (a) preferred. P(NO ₂) = 2.1 torr. P(Total) = 100 torr.	EX	292	(1.1±0.3)(11)			2
OH + CH₃CH₂CH₂OH → products						
Hydroxyl + 1-Propanol						
76 CAM/MCL	EX	292	(2.3±0.2)(12)			2
78 OVE/PAR1 Flash-photolysis. Resonance-absorption.	EX	296	(3.21±0.32)(12)			2
OH + (CH₃)₂CHOH → products						
Hydroxyl + 2-Propanol						
76 LLO/DAR1 k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.	RL	305	1.4(-1)			2/2
76 LLO/DAR1	RN	305	(4.3±1.3)(12)			2
78 OVE/PAR1 Flash-photolysis. Resonance-absorption.	EX	296	(3.30±0.33)(12)			2
OH + CH₂=CHCN → products						
Hydroxyl + 2-Propenenitrile (Acrylonitrile)						
81 HAR/KLE OH produced by UV photolysis of H ₂ O under flow conditions. Resonance-fluorescence.	EX	298-424	(2.43±0.03)(12)	0	0	2
OH + CH₃CH₂CN → products						
Hydroxyl + Propanenitrile						
81 HAR/KLE OH produced by UV photolysis of H ₂ O under flow conditions. Resonance-fluorescence.	EX	298-424	1.62(11)	0	800±176	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	E, B-B(ref)	k, A k err. units factor
OH + (CH₃)₃N → products						
Hydroxyl + Methanamine, N,N-dimethyl-						
78 ATK/PER3	EX	298-426	1.58(13)	0	-252±151	2
Flash-photolysis.						
Resonance-fluorescence.						
OH + CH₃CH₂CH₂ONO → products						
Hydroxyl + Nitrous acid propyl ester						
82 AUD/BAU1	EX	295	(1.56±0.32)(12)			2
Static system. OH generated by the chain reaction:						
$\text{H}_2\text{O}_2 + \text{NO}_2 + \text{CO}.$ $[\text{CH}_3\text{CH}_2\text{CH}_2\text{ONO}]_0 < 3.6 \times 10^{17} \text{ molec.cm}^{-3}.$ $[\text{H}_2\text{O}_2]_0 \sim 9.0 \times 10^{15} \text{ molec.cm}^{-3}.$ $[\text{NO}_2]_0 \sim 3.3 \times 10^{16} \text{ molec.cm}^{-3}.$ $[\text{CO}]_0 \sim 3.0 \times 10^{18} \text{ molec.cm}^{-3}.$ $P < 75 \text{ torr}.$						
OH + (CH₃)₂CHONO₂ → products						
Hydroxyl + Nitric acid 1-methylethyl ester (Isopropyl nitrate)						
82 ATK/ASC5 ¹⁾	RL	299	(2.4±0.6)(-2)			2/2
k _{ref} : OH +  → products.						
82 ATK/ASC5 ¹⁾	RN	299	(1.08±0.30)(11)			2
¹⁾ Photolysis of CH ₃ ONO/NO/Isopropyl nitrate.						
[CH ₃ ONO] ₀ = (0.9-7.1)×10 ¹⁴ molec.cm ⁻³ .						
[Alkyl nitrate] = 2.4×10 ¹³ molec.cm ⁻³ .						
OH + CH≡CC≡CH → CH≡CCH=C=O + H						
Hydroxyl + 1,3-Butadiyne						
82 BIT/HOW	ES	1700-1900	(5.0±2.0)(12)	0	0	2
C ₆ H ₆ /O ₂ /Ar flame. P = 20 torr.						
OH + CH₂=CHCH=CH₂ → products						
Hydroxyl + 1,3-Butadiene						
76 LLO/DAR2	RL	305	2.58(1)			2/2
k _{ref} : OH + CH ₃ CH ₂ CH ₂ CH ₃ → products.						
76 LLO/DAR2	RN	305	(4.64±0.93)(13)			2
77 ATK/PER3	EX	299-424	8.73(12)	0	-468±151	2
77 ATK/PER3	EX	299	(4.13±0.42)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
OH + CH ₃ CH ₂ CH=CH ₂ → H ₂ O + CH ₃ CHCH=CH ₂ (a)							
→ CH ₃ CH ₂ CH(OH)CH ₂ (b)							
→ CH ₃ CH ₂ CHCH ₂ OH (c)							
→ any other products (d)							
Hydroxyl + 1-Butene							
82 BIE/HAR ¹⁾ k _a /(k _a + k _b + k _c).	RL	298	(2.0±0.6)(-1)				2/2
82 BIE/HAR ¹⁾ k _a + k _b + k _c .	EX	298	(1.81±0.24)(13)				2
¹⁾ Discharge-flow. OH generated by reacting H with NO ₂ . [OH] ₀ = (0.2-2.0)×10 ¹² molec.cm ⁻³ . P(Total) ~ 2 torr.							
71 MOR/NIK2 k _{overall} . k _{ref} : OH + CH ₃ CH=CH ₂ → products.	RL	300	2.4				2/2
75 ATK/PIT ²⁾ k _{overall} .	EX	297-425	4.58(12)	0	-468±151		2
75 ATK/PIT ²⁾ k _{overall} .	EX	298	(2.13±0.22)(13)				2
75 PAS/CAR k _{overall} . Expressed as nk. (n = stoichiometric factor.)	EX	300	(9.03±0.60)(12)				2
76 WU/JAP k _{overall} . Cylindrical Pyrex Reactor. k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products. P = 760 torr.	RL	303	5.2(-1)				2/2
77 DAV ³⁾ k _{overall} . M = He. P(He) = 3 torr.	EX	298	(1.78±0.11)(13)				2
77 DAV ³⁾ k _{overall} . M = He. P(He) = 200 torr.	EX	298	(1.77±0.08)(13)				2
78 PIT/ATK ³⁾ k _{overall} . P ~ (15-650) torr.	EX	298	(2.13±0.22)(13)				2
78 RAV/WAG ³⁾ k _{overall} . M = He. P(He) = 3 torr.	EX	298	(1.78±0.11)(13)				2
78 RAV/WAG ³⁾ k _{overall} . M = He. P(He) = 20 torr.	EX	298	(1.77±0.08)(13)				2
79 NIP/PAR ³⁾ k _{overall} .	EX	297	(2.01±0.15)(13)				2
³⁾ Flash-photolysis. Resonance-fluorescence.							
OH + cis-CH ₃ CH=CHCH ₃ → products							
Hydroxyl + 2-Butene, (Z)-							
71 MOR/NIK2 k _{ref} : OH + CH ₃ CH=CH ₂ → products.	RL	300	3.6				2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 ATK/PIT	EX	297-425	6.26(12)	0	-488±151	2	
75 ATK/PIT	EX	298	(3.23±0.32)(13)			2	
76 LLO/DAR2	RL	305	2.18(1)			2/2	
k_{ref} : OH + CH ₃ CH ₂ CH ₂ CH ₃ → products.							
76 LLO/DAR2	RN	305	(3.92±0.80)(13)			2	
76 WIN/LLO	RL	305	1.22			2/2	
k_{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.							
76 WIN/LLO	RN	305	(3.72±0.56)(13)			2	
77 DAV ¹)	EX	298	(2.60±0.24)(13)			2	
M = He. P(He) = 3 torr.							
77 DAV ¹)	EX	298	(2.57±0.15)(13)			2	
M = He. P(He) = 20 torr.							
¹) Flash-photolysis. Resonance-fluorescence.							
78 PIT/ATK	RN	298	(3.91±0.78)(13)			2	
Propene/Air irradiation.							
P(Total) = 1 atm.							
78 PIT/ATK	EX	298	(3.23±0.33)(13)			2	
Flash-photolysis. Resonance-fluorescence.							
P ~ (15-650) torr.							
78 RAV/WAG ²)	EX	298	(2.60±0.24)(13)			2	
M = He. P(He) = 3 torr.							
78 RAV/WAG ²)	EX	298	(2.57±0.15)(13)			2	
M = He. P(He) = 20 torr.							
²) Flash-photolysis. Resonance-fluorescence.							
OH + trans-CH ₃ CH=CHCH ₃ → products							
Hydroxyl + 2-Butene, (E)-							
71 MOR/NIK2	RL	300	4.2			2/2	
k_{ref} : OH + CH ₃ CH ₃ CH ₂ → products.							
75 ATK/PIT	EX	297-425	6.74(12)	0	-549±151	2	
75 ATK/PIT	EX	298	(4.21±0.42)(13)			2	
75 COX	RN	300	(6.38±1.63)(13)			2	
k expressed as αk							
with $\alpha \sim 1.7$							
75 PAS/CAR	EX	300	(7.23±6.02)(12)			2	
k expressed as nk.							
(n = stoichiometric factor.)							
76 WU/JAP	RL	303	1.3			2/2	
k_{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products.							
P = 760 torr.							
78 PIT/ATK	EX	298	(4.21±0.42)(13)			2	
Propene/air irradiation.							
P(Total) = 760 torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
OH + (CH ₃) ₂ C=CH ₂ → H ₂ O + CH ₂ =C(CH ₃)CH ₂ (a)							
→ (CH ₃) ₂ C(OH)CH ₂ (b)							
→ (CH ₃) ₂ CCH ₂ OH (c)							
Hydroxyl + 1-Propene, 2-methyl-							
78 BAK/BAL ¹⁾	ES	753	2.9(13)				2
k _a . Possibly an upper-limit.							
78 BAK/BAL ¹⁾	RL	753	3.7				2/2
(k _b + k _c)/k _a .							
78 BAK/BAL ¹⁾	ES	753	7.8(12)				2 2.0
k _b + k _c .							
1) Oxidation in aged boric-acid-coated vessels.							
P(Total) = (490-505) torr.							
71 MOR/NIK2	RL	300	3.8				2/2
k _{overall} /k _{ref} .							
k _{ref} : OH + CH ₃ CH=CH ₂ → products.							
75 ATK/PIT ²⁾	EX	297-425	5.54(12)	0	-503±151		2
75 ATK/PIT ²⁾	EX	298	(3.05±0.31)(13)				2
2) k _{overall} .							
76 WU/JAP	RL	303	9.2(-1)				2/2
k _{overall} /k _{ref} . P = 760 torr.							
k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products.							
78 PIT/ATK	EX	298	(3.05±0.31)(13)				2
k _{overall} . Flash-photolysis.							
Resonance-fluorescence. P ~ (15-650) torr.							
OH + → H ₂ O + ^o							
Hydroxyl + Cyclobutane							
74 GOR/VOL ¹⁾	RL	298	8.47				2/2
74 GOR/VOL ¹⁾	RN	298	7.83(11)				2
1) Uncorrected for n-Butane impurity.							
74 GOR/VOL	RN	298	(7.23±1.81)(11)				2
Corrected for n-Butane impurity.							
OH + CH ₃ CH ₂ CH ₂ CH ₃ → H ₂ O + CH ₃ CH ₂ CH ₂ CH ₂ (a)							
→ H ₂ O + CH ₃ CH ₂ CHCH ₃ (b)							
Hydroxyl + Butane							
71 BAK/BAL	RL	753	5.25				2/2
k _a /k _{ref} . k _{ref} : OH + H ₂ → H ₂ O + H. Estimated ratio per primary CH bond.							
79 BAL/WAL1	RL	753-773	1.28	0	-1070		2/2
k _a /k _{ref} . k _{ref} : OH + H ₂ → H ₂ O + H. A and B recalculated from a given empirical formula.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
71 BAK/BAL k_b/k_{ref} . k_{ref} : $OH + H_2 \rightarrow H_2O + H$. Estimated ratio per secondary CH bond.	RL	753	1.175(1)			2/2
79 BAL/WAL1 k_b/k_{ref} . k_{ref} : $OH + H_2 \rightarrow H_2O + H$. A and B recalculated from given empirical formula.	RL	753-773	6.92(-1)	0	-1820	2/2
71 BAK/BAL $(k_a + k_b)/k_{ref}$. k_{ref} : $OH + H_2 \rightarrow H_2O + H$.	RL	753	(3.40±0.34)(1)			2/2
71 MOR/NIK2 $(k_a + k_b)/k_{ref}$. k_{ref} : $OH + CH_3CH=CH_2 \rightarrow$ products.	RL	300	2.4(-1)			2/2
74 GOR/VOL $(k_a + k_b)/k_{ref}$. k_{ref} : $OH + CO \rightarrow H + CO_2$.	RL	298	1.94(1)			2/2
75 CAM/HAN1 $(k_a + k_b)/k_{ref}$. k_{ref} : $OH + CO \rightarrow H + CO_2$	RL	292	(1.48±0.09)(1)			2/2
75 HUC/BOO $(k_a + k_b)/k_{ref}$. k_{ref} : $OH + CH_3CH_2CH_3 \rightarrow H_2O + CH_3CH_2CH_2$ (C) $\rightarrow H_2O + (CH_3)_2CH$ (d)	RL	653	(1.54±0.13)			2/2
82 ATK/ASC2 1) $(k_a + k_b)/k_{ref}$. k_{ref} : $OH + CH_3(CH_2)_4CH_3 \rightarrow$ products.	RL	299	(4.53±0.07)(-1)			2/2
82 ATK/ASC2 1) $(k_a + k_b)/k_{ref}$. k_{ref} : $OH +$  $\rightarrow$ products.	RL	299	(3.41±0.02)(-1)			2/2
73 GOR 2) 73 STU2 2) 74 GOR/VOL 2) 75 GOR/MUL1 2) M = Ar (710 torr.) + H ₂ O (10 torr.) + C ₄ H ₁₀ (0.54-2.46 torr.)	EX	298	(1.97±0.05)(12)			2
75 GOR/MUL1 2) P = (0.5-198) torr. In an atmosphere of water vapor.	EX	298	(1.42±0.21)(12)			2
75 GOR/MUL1 2) P = (0.5-198) torr. In an atmosphere of water vapor.	RN	298	(1.75±0.42)(12)			2
75 GOR/MUL1 2) P = (0.5-198) torr. In an atmosphere of water vapor.	EX	298	(2.54±0.1)(12)			2
75 GOR/MUL1 2) P = (0.5-198) torr. In an atmosphere of water vapor.	EX	381	(2.5±0.1)(12)			2
75 GOR/MUL1 2) P = (0.5-198) torr. In an atmosphere of water vapor.	EX	416	(3.0±0.1)(12)			2
76 PER/ATK2 2) 76 PER/ATK2 2) 80 PAR/NIP 2) Flash-photolysis. Resonance-absorption.	EX	297-420	1.06(13)	0	559±151	2
	EX	297	(1.64±0.16)(12)			2
	EX	297	(1.61±0.13)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 ATK/ASC2 1) 2) Mean of four previously reported k's. 1) CH ₃ ONO/NO/CH ₃ CH ₂ CH ₂ CH ₃ /Cyclohexane (or Hexane) photolysis. [CH ₃ ONO] ₀ = (9.5-3.5) × 10 ¹⁴ molec.cm ⁻³ . [Butane] = (1.2-2.4) × 10 ¹³ molec.cm ⁻³ . P(Total) = 735 torr.	SE	299	1.55(12)			2
82 AUD/BAU1 2) Static system. OH generated by the chain reaction: H ₂ O ₂ + NO ₂ + CO. P < 75 torr. [CO] ₀ ~ 3.0 × 10 ¹⁸ molec.cm ⁻³ . [Butane] ₀ < 3.6 × 10 ¹⁷ molec.cm ⁻³ . [H ₂ O ₂] ₀ ~ 9.0 × 10 ¹⁵ molec.cm ⁻³ . [NO ₂] ₀ ~ 3.3 × 10 ¹⁶ molec.cm ⁻³ . 2) k _a + k _b .	EX	295	(1.63 ± 0.16)(12)			2
OH + CD ₃ CD ₂ CD ₂ CD ₃ → HDO + CD ₃ CD ₂ CD ₂ CD ₂ (a) → HDO + CD ₃ CD ₂ CD ₂ CD ₃ (b) Hydroxyl + Butane-d ₁₀						
80 PAR/NIP k _a + k _b . Flash-photolysis. Resonance-absorption.	EX	297	(4.20 ± 0.41)(11)			2
OD + CH ₃ CH ₂ CH ₂ CH ₃ → HDO + CH ₃ CH ₂ CH ₂ CH ₂ (a) → HDO + CH ₃ CH ₂ CHCH ₃ (b) Hydroxyl-d + Butane						
80 PAR/NIP k _a + k _b . Flash-photolysis. Resonance-absorption.	EX	297	(1.66 ± 0.13)(12)			2
OD + CD ₃ CD ₂ CD ₂ CD ₃ → D ₂ O + CD ₃ CD ₂ CD ₂ CD ₂ (a) → D ₂ O + CD ₃ CD ₂ CD ₂ CD ₃ (b) Hydroxyl-d + Butene-d ₁₀						
80 PAR/NIP k _a + k _b . Flash-photolysis. Resonance-absorption.	EX	297	(4.84 ± 0.38)(11)			2
OH + (CH ₃) ₃ CH → H ₂ O + (CH ₃) ₃ C (a) → H ₂ O + (CH ₃) ₂ CHCH ₃ (b) Hydroxyl + Propane, 2-methyl-						
71 BAK/BAL k _a . Rate constant per tertiary CH bond.	CO	298-753	5.3(13)	0	1203	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
71 BAK/BAL k_a/k_{ref} . k_{ref} : $OH + H_2 \rightarrow H_2O + H$. Estimated ratio per tertiary CH bond.	RL	753	1.525(1)			2/2
72 GOR/VOL k_a/k_{ref} . k_{ref} : $OH + CO \rightarrow H + CO_2$	RL	298	(2.33±0.07)(1)			2/2
72 GOR/VOL k_a . Similar data in 72 VOL/GOR and 73 GOR.	RN	298	(2.11±0.48)(12)			2
78 DAR/ATK k_a . Irradiation technique. Computed from an empirical formula.	CO	300	1.26(12)			2
79 BAL/WAL1 1) k_a/k_{ref} . A and B recalculated from a given empirical formula. k_{ref} : $OH + H_2 \rightarrow H_2O + H$.	RL	753-773	2.73(-1)	0	-2060	2/2
81 BAL/WAL2 1) k_a . 1) Oxidation of 2,2,3-Trimethylbutane in H_2/O_2 mixtures in aged boric-acid-coated vessels. Gas-chromatography. P(Total) = 500 torr. P(2,2,3-Trimethylbutane) = 5 torr.	ES	300-1500	2.57(12)	0	271±96	2 1.2
71 BAK/BAL k_b/k_{ref} . k_{ref} : $OH + H_2 \rightarrow H_2O + H$. Estimated ratio per primary CH bond.	RL	753	5.25			2/2
78 DAR/ATK k_b . Irradiation technique. Computed from an empirical formula.	CO	300	3.5(11)			2
79 BAL/WAL1 k_b/k_{ref} . A and B recalculated from an empirical formula. k_{ref} : $OH + H_2 \rightarrow H_2O + H$.	RL	753-773	1.93	0	-1070	2/2
71 BAK/BAL $(k_a + k_b)/k_{ref}$. k_{ref} : $OH + H_2 \rightarrow H_2O + H$.	RL	753	(3.10±0.31)(1)			2/2
75 HUC/BOO $(k_a + k_b)/k_{ref}$. k_{ref} : $OH + CH_3CH_2CH_3 \rightarrow H_2O + (CH_3)_2CH$ (c) $\rightarrow H_2O + CH_3CH_2CH_2$ (d)	RL	653	(1.28±0.07)			2/2
76 WU/JAP $(k_a + k_b)/k_{ref}$. Pyrex Reactor. P = 760 torr. k_{ref} : $OH + cis-CH_3CH=CHCH_3 \rightarrow$ products.	RL	303	4.0(-2)			2/2
78 BUT/SOL $k_a + k_b$. Quartz reactor. H_2O_2 photolysis. Gas-chromatography. P($O_2 + N_2$) > 100 torr.	RN	305	(9.58±1.08)(11)			2
78 DAR/ATK $k_a + k_b$. Irradiation technique.	EX	300	(1.53±0.03)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{OH} + \text{C}_4\text{H}_4\text{O} \rightarrow \text{products}$ Hydroxyl + Furan 82 LEE/TAN Discharge-flow. Resonance-fluorescence. OH generated by reacting H with NO_2 .	EX	295	(6.32±0.48)(13)			2
$\text{OH} + \text{CH}_3\text{CH}=\text{CHCHO} \rightarrow \text{products}$ Hydroxyl + 2-Butenal (Crotonaldehyde) 81 KER/SHE ¹⁾ $k_{\text{ref}}: \text{OH} + \text{CH}_2=\text{CH}_2 \rightarrow \text{products}$. 81 KER/SHE ¹⁾ ¹⁾ Photolysis of HONO/Synthetic air mixtures containing low concentrations of Ethene and aldehyde.	RL	298	(4.12±0.80)			2/2
$\text{OH} + \text{CH}_3\text{C}(\text{O})\text{CH}=\text{CH}_2 \rightarrow \text{products}$ Hydroxyl + 3-Buten-2-one 80 COX/DER1 HONO photosensitized oxidation in synthetic air. Gas-chromatography. Same data given in 80 COX. $[\text{NO}] = [\text{NO}_2] = (0.3-3.0) \text{ ppm}$. $[\text{HONO}] = (3-20) \text{ ppm}$. 82 KLE/HAR $\text{M} = \text{Ar}$. OH generated by photolysis of water vapor. Flash-photolysis. Resonance-fluorescence. $\text{P}(\text{Total}) = 50 \text{ torr}$.	RN	300	8.43(12)			2
$\text{OH} + \text{CH}_2=\text{C}(\text{CH}_3)\text{CHO} \rightarrow \text{products}$ Hydroxyl + 2-Propenal, 2-methyl- (Methacrolein) 82 KLE/HAR $\text{M} = \text{Ar}$. OH generated by Photolysis of Water vapor. Flash-photolysis. Resonance-fluorescence. $\text{P}(\text{Total}) = 50 \text{ torr}$.	EX	297-424	1.07(13)	0	-456±73	2
$\text{OH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHO} \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CO}$ (a) $\rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}_2\text{CHCHO}$ (b) $\rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CHCH}_2\text{CHO}$ (c) $\rightarrow \text{H}_2\text{O} + \text{CH}_2\text{CH}_2\text{CH}_2\text{CHO}$ (d) Hydroxyl+ Butanal 81 AUD/BAU ¹⁾ $(k_a + k_b + k_c + k_d)/k_{\text{ref}}$. $k_{\text{ref}}: \text{OH} + \text{CH}_3\text{CHO} \rightarrow \text{products}$.	RL	298	(1.62±0.20)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 AUD/BAU ¹⁾ k _a + k _b + k _c + k _d . ¹⁾ Linear, boric-acid-coated flow tube. Gas-chromatography. Channel (a) is predominant. P(Total) = 299 torr.	RN	298	(1.52±0.19)(13)			2
81 KER/SHE ²⁾ k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(2.96±0.07)			2/2
81 KER/SHE ²⁾ ²⁾ Photolysis of HONO/Synthetic air mixtures containing low concentrations of Ethene and aldehyde.	EX	298	(1.45±0.06)(13)			2
OH + (CH ₃) ₂ CHCHO → H ₂ O + (CH ₃) ₂ CHCO (a) → H ₂ O + (CH ₃) ₂ CHCHO (b) → H ₂ O + CH ₂ CH(CH ₃)CHCHO (c)						
Hydroxyl + Propanal, 2-methyl-						
79 BAL/CLE k _b /k _a . Oxidation in an aged boric-acid-coated vessel. P(Total) = 60 torr.	RL	713	(7.0±1.0)(-1)			2
81 AUD/BAU ¹⁾ (k _a + k _b + k _c)/k _{ref} . k _{ref} : OH + CH ₃ CHO → products.	RL	298	(1.12±0.13)			2/2
81 AUD/BAU ¹⁾ k _a + k _b + k _c . ¹⁾ Linear, boric-acid-coated flow tube. Gas-chromatography. Channel (a) is predominant. P(Total) = 299 torr.	RN	298	(1.05±0.12)(13)			2
81 KER/SHE ²⁾ (k _a + k _b + k _c)/k _{ref} . k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(3.40±0.66)			2/2
81 KER/SHE ²⁾ k _a + k _b + k _c . ²⁾ HONO/Synthetic air/Ethene/aldehyde photolysis.	RN	298	(1.63±0.06)(13)			2
OH + CH ₃ C(O)CH ₂ CH ₃ → products						
Hydroxyl + 2-Butanone						
76 WIN/LLO k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.	RL	305	7.0(-2)			2/2
76 WIN/LLO	RN	305	(2.0±0.6)(12)			2
80 COX/DER1 HONO photosensitized oxidation in synthetic air. Gas chromatography. Same data given in 80 COX. [NO] = NO ₂ = (0.3-3.0) ppm. [HONO] = (3-20) ppm.	RN	300	1.57(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 COX/PAT ¹⁾ k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	296	(0.11±0.01)			2/2
81 COX/PAT ¹⁾ ¹⁾ Photolysis of HONO diluted N ₂ /O ₂ mixtures, in presence of Butane. P = 760 torr.	RN	296	(5.30±0.54)(11)			2
OH + CH ₃ CH ₂ CH ₂ COOH → products Hydroxyl + Butanoic acid						
82 ZET/STU Pulsed vacuum UV-Photolysis of H ₂ O, Ar and Butanoic acid mixtures. Resonance-fluorescence. P(Ar) = (30-300) torr. P(H ₂ O) = (0.04-0.1) torr.	EX	298	(1.08±0.10)(12)			2
OH + CH ₃ C(O)OCH ₂ CH ₃ → products Hydroxyl + Acetic acid ethyl ester (Ethyl acetate)						
78 CAM/PAR Reaction of ester vapor with OH. Vacuum system. OH generated by reaction of a H ₂ O ₂ /NO ₂ /CO mixture. P(Total) = 100 torr. P(NO ₂) = 2.1 torr.	EX	292	(1.16±0.13)(12)			2
OH + CH ₃ CH ₂ C(O)OCH ₃ → products Hydroxyl + Propanoic acid methyl ester						
78 CAM/PAR Reaction of ester vapor with OH. Vacuum system. OH generated by reaction of a H ₂ O ₂ /NO ₂ /CO mixture. P(Total) = 100 torr. P(NO ₂) = 2.1 torr.	EX	292	(1.7±0.6)(11)			2
OH +  → products Hydroxyl + Furan, tetrahydro-						
77 WIN/LLO k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.	RL	305	2.9(-1)			2/2
77 WIN/LLO	RN	305	(8.8±1.8)(12)			2
78 RAV/DAV ¹⁾ M = He. P(He) = 20 torr.	EX	298	(9.82±0.96)(12)			2
78 RAV/DAV ¹⁾ M = He. P(He) = 200 torr.	EX	298	(9.58±2.35)(12)			2
¹⁾ Flash-photolysis. Resonance-fluorescence.						
OH + CH ₃ CH ₂ CH ₂ CH ₂ OH → products Hydroxyl + 1-Butanol						
76 CAM/MCL	EX	292	(4.1±0.6)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + (CH₃CH₂)₂O → products						
Hydroxyl + Ethane, 1,1'-oxybis-						
76 LLO/DAR1	RL	305	1.85(-1)			2/2
k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.						
76 LLO/DAR1	RN	305	(5.6±1.1)(12)			2
OH + (CH₃)₃COOH → products						
Hydroxyl + Hydroperoxide, 1,1-dimethylethyl-						
78 ANA/SMI2	EX	298	(1.81±0.48)(12)			2
Flash-photolysis of (CH ₃) ₃ COOH/H ₂ O mixtures.						
[(CH ₃) ₃ COOH] = (0.8-2.0)×10 ¹⁵ molec.cm ³ .						
[H ₂ O] = ~1.5×10 ¹⁶ molec.cm ³ .						
OH +  → products						
Hydroxyl + Thiophene						
82 LEE/TAN	EX	295	(2.87±0.38)(13)			2
Discharge-flow. Resonance-fluorescence.						
OH generated by reacting H with NO ₂ .						
OH + CH₃CH₂CH₂CH₂ONO → products						
Hydroxyl + Nitrous acid butyl ester (n-Butyl nitrite)						
82 AUD/BAU1	EX	295	(3.41±1.48)(12)			2
Static system. OH generated by the chain reaction:						
H ₂ O ₂ + NO ₂ + CO.						
P < 75 torr. [CO] ₀ ~ 3.0×10 ¹⁸ molec.cm ⁻³ .						
[CH ₃ (CH ₂) ₃ ONO] ₀ < 3.6×10 ¹⁷ molec.cm ⁻³ .						
[H ₂ O ₂] ₀ ~ 9.0×10 ¹⁵ molec.cm ⁻³ .						
[NO ₂] ₀ ~ 3.3×10 ¹⁶ molec.cm ⁻³ .						
OH + CH₃CH₂CH(CH₃)ONO → products						
Hydroxyl + Nitrous acid 1-methylpropyl ester						
(s-Butyl nitrite)						
82 AUD/BAU1	EX	295	(3.89±0.58)(12)			2
Static system. OH generated by the chain reaction:						
H ₂ O ₂ + NO ₂ + CO.						
[CH ₃ CH ₂ CH(CH ₃)ONO] ₀ < 3.6×10 ¹⁷ molec.cm ⁻³ .						
P < 75 torr. [CO] ₀ ~ 3.0×10 ¹⁸ molec.cm ⁻³ .						
[H ₂ O ₂] ₀ ~ 9.0×10 ¹⁵ molec.cm ⁻³ .						
[NO ₂] ₀ ~ 3.3×10 ¹⁶ molec.cm ⁻³ .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + (CH₃)₂CHCH₂ONO → products						
Hydroxyl + Nitrous acid 2-methylpropyl ester (iso-Butyl nitrite)						
82 AUD/BAU1	EX	295	(3.47±0.52)(12)			2
Static system. OH generated by the chain reaction: $\text{H}_2\text{O}_2 + \text{NO}_2 + \text{CO}$. P < 75 torr. $[\text{CO}]_0 \sim 3.0 \times 10^{18}$ molec.cm ⁻³ . $[(\text{CH}_3)_2\text{CHCH}_2\text{ONO}]_0 < 3.6 \times 10^{17}$ molec.cm ⁻³ . $[\text{H}_2\text{O}_2]_0 \sim 9.0 \times 10^{15}$ molec.cm ⁻³ . $[\text{NO}_2]_0 \sim 3.3 \times 10^{16}$ molec.cm ⁻³ .						
OH + (CH₃)₃CONO → products						
Hydroxyl + Nitrous acid 1,1-dimethylethyl ester (t-Butyl nitrite)						
82 AUD/BAU1	EX	295	(9.1±1.5)(11)			2
Static system. OH generated by the chain reaction: $\text{H}_2\text{O}_2 + \text{NO}_2 + \text{CO}$. P < 75 torr. $[\text{CO}]_0 \sim 3.0 \times 10^{18}$ molec.cm ⁻³ . $[(\text{CH}_3)_3\text{CONO}]_0 < 3.6 \times 10^{17}$ molec.cm ⁻³ . $[\text{H}_2\text{O}_2]_0 \sim 9.0 \times 10^{15}$ molec.cm ⁻³ . $[\text{NO}_2]_0 \sim 3.3 \times 10^{16}$ molec.cm ⁻³ .						
OH + CH₃CH₂CH₂CH₂ONO₂ → products						
Hydroxyl + Nitric acid butyl ester (n-Butyl nitrate)						
82 ATK/ASC5 ¹⁾	RL	299	(1.87±0.14)(-1)			2/2
k _{ref} : OH +  → products.						
82 ATK/ASC5 ¹⁾	RN	299	(8.55±0.66)(11)			2
¹⁾ CH ₃ ONO/NO/n-Butyl nitrate photolysis. $[\text{CH}_3\text{ONO}]_0 = (0.9-7.1) \times 10^{14}$ molec.cm ⁻³ . [n-Butyl nitrate] = 2.4 × 10 ¹³ molec.cm ⁻³ .						
OH + CH₃CH₂CH(CH₃)ONO₂ → products						
Hydroxyl + Nitric acid 1-methylpropyl ester (s-Butyl nitrate)						
82 ATK/ASC5 ¹⁾	RL	299	(9.1±1.3)(-2)			2/2
k _{ref} : OH +  → products.						
82 ATK/ASC5 ¹⁾	RN	299	(4.15±0.60)(11)			2
¹⁾ CH ₃ ONO/NO/s-Butyl nitrate photolysis. $[\text{CH}_3\text{ONO}]_0 = (0.9-7.1) \times 10^{14}$ molec.cm ⁻³ . [s-Butyl nitrate] = 2.4 × 10 ¹³ molec.cm ⁻³ .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
OH + (CH₃CH₂)₂NOH → H₂O + [C₄H₁₀NO]							
Hydroxyl + Ethanamine, N-ethyl-N-hydroxy-							
77 GOR/LII Electron pulse. P(Total) = 760 torr.	EX	308	6.1(13)			2	
OH + CH₂=C(CH₃)CH=CH₂ → products							
Hydroxyl + 1,3-Butadiene-, 2-methyl- (Isoprene)							
80 COX/DER1 HONO photosensitized oxidation in synthetic air. Gas-chromatography. Same data given on 80 COX. [NO] = NO ₂ = (0.3-3.0) ppm. [HONO] = (3-20) ppm.	RN	300	4.46(13)			2	
82 ATK/ASC2 ¹⁾ k _{ref} : OH + CH ₃ CH=CH ₂ → products.	RL	299	(3.81±0.17)			2/2	
82 ATK/ASC2 ¹⁾ ¹⁾ CH ₃ ONO/NO/Isoprene/Propene photolysis. [CH ₃ ONO] ₀ = (9.5-3.5)×10 ¹⁴ molec.cm ⁻³ . [Isoprene] = (1.2-2.4)×10 ¹³ molec.cm ⁻³ . P(Total) = 735 torr.	RN	299	(5.78±0.20)(13)			2	
82 KLE/HAR OH generated by flash-photolysis of H ₂ O in Ar. Resonance-fluorescence. P(Total) = 50 torr.	EX	297-424	1.42(13)	0	-409±27	2	
OH + CH₃CH₂CH₂CH=CH₂ → H₂O + CH₃CH₂CHCH=CH₂ (a)							
→ CH ₃ CH ₂ CH ₂ CH(OH)CH ₂ (b)							
→ CH ₃ CH ₂ CH ₂ CHCH ₂ OH (c)							
Hydroxyl + 1-Pentene							
82 BIE/HAR ¹⁾ k _a /(k _a + k _b + k _c).	RL	298	(1.3±0.5)(-1)			2/2	
82 BIE/HAR ¹⁾ k _a /(k _a + k _b + k _c). P(Total) ~ 2 torr.(Ar)	EX	298	(1.75±0.24)(13)			2	
82 BIE/HAR ¹⁾ k _a /(k _a + k _b + k _c). P(Total) = 50 torr.(Ar)	EX	298	(1.73±0.08)(13)			2	
¹⁾ Discharge-flow. OH generated by reacting H with NO ₂ . [OH] ₀ = (0.2-2.0)×10 ¹² molec.cm ⁻³ .							
71 MOR/NIK2 k _{overall} . k _{ref} : CH ₃ CH=CH ₂ + OH → products.	RL	300	2.5			2/2	
76 WU/JAP k _{overall} . Pyrex Reactor. P = 760 torr. k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products.	RL	303	5.6(-1)			2/2	
79 NIP/PAR k _{overall} . Flash-photolysis. Resonance-fluorescence.	EX	297	(2.39±0.23)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, . B-B(ref)	k, A k err. units factor
OH + CH₃CH₂CH=CHCH₃ → products						
Hydroxyl + 2-Pentene (Unspecified form)						
71 MOR/NIK2	RL	300	5.3			2/2
k _{ref} : OH + CH ₃ CH=CH ₂ → products.						
OH + cis-CH₃CH₂CH=CHCH₃ → products						
Hydroxyl + 2-Pentene, (Z)-						
76 WU/JAP	RL	303	1.2			2/2
Cylindrical Pyrex Reactor. P = 760 torr.						
k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products.						
OH + CH₃CH₂C(CH₃)=CH₂ → products						
Hydroxyl + 1-Butene, 2-methyl-						
71 MOR/NIK2	RL	300	5.3			2/2
k _{ref} : OH + CH ₃ CH=CH ₂ → products.						
76 WU/JAP	RL	303	1.1			2/2
Cylindrical Pyrex Reactor. P = 760 torr.						
k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products.						
OH + (CH₃)₂CHCH=CH₂ → products						
Hydroxyl + 1-Butene, 3-methyl-						
77 ATK/PER3	EX	299-424	3.15(12)	0	-533±151	2
77 ATK/PER3	EX	299	(1.87±0.19)(13)			2
OH + (CH₃)₂C=CHCH₃ → products						
Hydroxyl + 2-Butene, 2-methyl-						
71 MOR/NIK2	RL	300	7.0			2/2
k _{ref} : OH + CH ₃ CH=CH ₂ → products.						
76 ATK/PER1	EX	297-425	2.217(13)	0	-226±201	2
76 ATK/PER1	EX	298	(4.70±0.48)(13)			2
78 ATK/PIT2	EX	299-441	1.15(13)	0	-450±15 1	2
Flash-photolysis. NO ₂ chemiluminescence.						
78 PIT/ATK	EX	298	(4.70±0.54)(13)			2
Flash-photolysis. Resonance-fluorescence.						
P ~ (15-650) torr.						
82 ATK/ASC2 ¹⁾	RL	299	(3.43±0.13)			2/2
k _{ref} : OH + CH ₃ CH=CH ₂ → products.						
82 ATK/ASC2 ¹⁾	RN	299	(5.20±0.20)(13)			2
¹⁾ CH ₃ ONO/NO/2-Methyl-2-butene/Propane photolysis.						
[2-Methyl-2-butene] = (1.2-2.4)×10 ¹³ molec.cm ⁻³ .						
[CH ₃ ONO] ₀ = (9.5-3.5)×10 ¹⁴ molec.cm ⁻³ .						
P(Total) = 735 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH +  → products						
Hydroxyl + Cyclopentane						
82 ATK/ASC2 ¹⁾ k _{ref} : OH + CH ₃ (CH ₂) ₄ CH ₃ → products.	RL	299	(7.04±0.07)(-1)			2/2
82 ATK/ASC2 ¹⁾ ¹⁾ CH ₃ ONO/NO/Cyclohexane/Cyclopentane photolysis. [Cyclopentane] = (1.2-2.4)×10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (9.5-3.5)×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.	RN	299	(3.21±0.04)(12)			2
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ → H ₂ O + CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ (a) → H ₂ O + CH ₃ CH ₂ CH ₂ CHCH ₃ (b) → H ₂ O + CH ₃ CH ₂ CHCH ₂ CH ₃ (c)						
Hydroxyl + Pentane						
78 DAR/ATK k _a . Irradiation technique. Computed from an empirical formula.	CO	300	2.35(11)			2
79 BAL/WAL1 k _a /k _{ref} . A and B recalculated from a given empirical formula. k _{ref} : OH + H ₂ → H ₂ O + H.	RL	753-773	1.28	0	-1070	2/2
78 DAR/ATK k _b . Irradiation technique. Computed from an empirical formula.	CO	300	1.40(12)			2
79 BAL/WAL1 k _b /k _{ref} . A and B recalculated from a given empirical formula. k _{ref} : OH + H ₂ → H ₂ O + H.	RL	753-773	6.92(-1)	0	-1820	2/2
78 DAR/ATK k _c . Irradiation technique. Computed from an empirical formula.	CO	300	6.99(11)			2
79 BAL/WAL1 k _c /k _{ref} . A and B recalculated from a given empirical formula. k _{ref} : OH + H ₂ → H ₂ O + H.	RL	753-773	3.46(-1)	0	-1820	2/2
76 WU/JAP k _a + k _b + k _c . Cylindrical Pyrex Reactor. k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products. P = 760 torr.	RL	303	1.2(-1)			2/2
78 DAR/ATK k _a + k _b + k _c . Irradiation technique.	EX	300	(2.25±0.08)(12)			2
80 COX/DER1	RN	300	3.01(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$k_a + k_b + k_c$. HONO photosensitized oxidation in synthetic air. $[\text{NO}] = [\text{NO}_2] = (0.3\text{--}3.0)$ ppm. $[\text{HONO}] = (3\text{--}20)$ ppm. Same data given in 80 COX.						
82 ATK/ASC3 ¹⁾ $(k_a + k_b + k_c)/k_{\text{ref}}$. k_{ref} : $\text{OH} + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{products}$.	RL	299	$(4.53 \pm 0.07)(-1)$			2/2
82 ATK/ASC3 ¹⁾ $k_a + k_b + k_c$.	RN	299	$(2.49 \pm 0.05)(12)$			2
¹⁾ Photolysis of $\text{CH}_3\text{ONO}/\text{NO}/\text{Pentane}$ mixtures. $[\text{CH}_3\text{ONO}]_0 = (2.1\text{--}4.0) \times 10^{14}$ molec. cm^{-3} . $[\text{Pentane}] = (1.2\text{--}2.4) \times 10^{13}$ molec. cm^{-3} . $P(\text{Total}) = 735$ torr.						
$\text{OH} + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ (a) $\rightarrow \text{H}_2\text{O} + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2$ (b) $\rightarrow \text{H}_2\text{O} + (\text{CH}_3)_2\text{CHCHCH}_3$ (c) $\rightarrow \text{H}_2\text{O} + (\text{CH}_3)_2\text{CCH}_2\text{CH}_3$ (d)						
Hydroxyl + Butane, 2-methyl- (Isopentane)						
78 DAR/ATK ¹⁾ k_a .	CO	300	2.35(11)			2
78 DAR/ATK ¹⁾ k_b .	CO	300	1.17(11)			2
78 DAR/ATK ¹⁾ k_c .	CO	300	6.99(11)			2
78 DAR/ATK ¹⁾ k_d .	CO	300	1.26(12)			2
¹⁾ Irradiation. k computed from an empirical formula.						
79 BAL/WAL1 ²⁾ k_a/k_{ref} .	RL	753-773	1.28	0	-1070	2/2
79 BAL/WAL1 ²⁾ k_b/k_{ref} .	RL	753-773	6.42(-1)	0	-1070	2/2
79 BAL/WAL1 ²⁾ k_c/k_{ref} .	RL	753-773	3.46(-1)	0	-1820	2/2
79 BAL/WAL1 ²⁾ k_d/k_{ref} .	RL	753-773	2.73(-1)	0	-2060	2/2
²⁾ A and B recalculated from a empirical formula.						
k_{ref} : $\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$.						
76 LLO/DAR2 $(k_a + k_b + k_c + k_d)/k_{\text{ref}}$. k_{ref} : $\text{OH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{products}$.	RL	305	1.10			2/2
76 LLO/DAR2 $k_a + k_b + k_c + k_d$	RN	305	$(2.0 \pm 0.4)(12)$			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
78 DAR/ATK $k_a + k_b + k_c + k_d$. Irradiation technique.	EX	300	(2.28±0.04)(12)			2
80 COX/DER1 $k_a + k_b + k_c + k_d$. HONO photosensitized oxidation in synthetic air. [NO] = [NO ₂] = (0.3-3.0) ppm. [HONO] = (3-20) ppm. Same data given in 80 COX.	RN	300	2.11(12)			2
OH + (CH ₃) ₄ C → H ₂ O + (CH ₃) ₃ CCH ₂						
Hydroxyl + Propane, 2,2-dimethyl- (Neopentane)						
71 BAK/BAL ¹⁾	RL	753	(1.60±0.16)(1)			2/2
76 BAK/BAL ¹⁾	RL	753	(1.0±0.1)(1)			2/2
¹⁾ k _{ref} : OH + H ₂ → H ₂ O + H.						
76 BAK/BAL	ES	753	(3.9±0.4)(12)			2
78 DAR/ATK ¹⁾	EX	300	(6.3±1.0)(11)			2
78 DAR/ATK ¹⁾	CO	300	4.70(11)			2
Calculation using an empirical formula.						
¹⁾ Irradiation technique.						
79 BAL/WAL1 A and B recalculated from a empirical formula. k _{ref} : OH + H ₂ → H ₂ O + H.	RL	753-773	2.57	0	-1070	2/2
80 PAR/NIP Flash-photolysis. Resonance-absorption.	EX	297	(5.48±0.59)(11)			2
82 ATK/ASC2 ¹⁾ k _{ref} : OH + CH ₃ (CH ₂) ₄ CH ₃ → products.	RL	299	(1.35±0.07)(-1)			2/2
82 ATK/ASC2 ¹⁾ ¹⁾ CH ₃ ONO/NO/Neopentane photolysis. [Neopentane] = (1.2-2.4)×10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (9.5-3.5)×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.	RN	299	(4.64±0.30)(11)			2
OH + CH ₃ CH ₂ CH ₂ CH ₂ CHO → H ₂ O + CH ₃ CH ₂ CH ₂ CH ₂ CO (a) → H ₂ O + CH ₃ CH ₂ CH ₂ CHCHO (b) → H ₂ O + CH ₃ CH ₂ CHCH ₂ CHO (c) → H ₂ O + CH ₃ CHCH ₂ CH ₂ CHO (d) → H ₂ O + CH ₂ CH ₂ CH ₂ CH ₂ CHO (e)						
Hydroxyl + Pentanal						
81 AUD/BAU ¹⁾ (k _a + k _b + k _c + k _d + k _e)/k _{ref} . k _{ref} : OH + CH ₃ CHO → products.	RL	298	(8.8±1.1)(-1)			2/2
81 AUD/BAU ¹⁾ k _a + k _b + k _c + k _d + k _e . ¹⁾ Linear, boric-acid-coated flow tube. Channel (a) is predominant. P(Total) = 299 torr.	RN	298	(8.3±1.0)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 KER/SHE ²) (k _a + k _b + k _c + k _d + k _e)/k _{ref} . k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(3.24±0.49)			2/2
81 KER/SHE ²) k _a + k _b + k _c + k _d + k _e . 2) HONO/Synthetic air/Ethene/aldehyde photolysis.	RN	298	(1.57±0.24)(13)			2
OH + (CH ₃) ₂ CHCH ₂ CHO → H ₂ O + (CH ₃) ₂ CHCH ₂ CO (a) → H ₂ O + (CH ₃) ₂ CHCHCHO (b) → H ₂ O + (CH ₃) ₂ CCH ₂ CHO (c) → H ₂ O + CH ₂ CH(CH ₃)CH ₂ CHO (d)						
Hydroxyl + Butanal, 3-methyl-						
81 AUD/BAU ¹) (k _a + k _b + k _c + k _d)/k _{ref} . k _{ref} : OH + CH ₃ CHO → products.	RL	298	(1.18±0.13)			2/2
81 AUD/BAU ¹) k _a + k _b + k _c + k _d . 1) Boric-acid-coated flow tube. Channel (a) is predominant. P(Total) = 299 torr.	RN	298	(1.11±0.12)(13)			2
81 KER/SHE ²) (k _a + k _b + k _c + k _d)/k _{ref} . k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(3.39±0.10)			2/2
81 KER/SHE ²) k _a + k _b + k _c + k _d . 2) HONO/Synthetic air/Ethene/aldehyde photolysis.	RN	298	(1.63±0.06)(13)			2
OH + (CH ₃) ₃ CCCHO → H ₂ O + (CH ₃) ₃ CCO (a) → H ₂ O + CH ₂ C(CH ₃) ₂ CHO (b)						
Hydroxyl + Propanal, 2,2-dimethyl-						
81 AUD/BAU ¹) (k _a + k _b)/k _{ref} . k _{ref} : OH + CH ₃ CHO → products.	RL	298	(5.4±0.6)(-1)			2/2
81 AUD/BAU ¹) k _a + k _b . 1) Boric-acid-coated flow tube. Channel (a) is predominant. P(Total) = 299 torr.	RN	298	(5.1±0.5)(12)			2
81 KER/SHE ²) (k _a + k _b)/k _{ref} . k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(2.63±0.73)			2/2
81 KER/SHE ²) k _a + k _b . 2) HONO/Synthetic air/Ethene/aldehyde photolysis.	RN	298	(1.26±0.36)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref)), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH ₃ C(O)CH ₂ CH ₂ CH ₃ → products Hydroxyl + 2-Pentanone 82 ATK/ASC4 ¹⁾	RL	299	(6.26±0.18)(-1)			2/2
k _{ref} : OH +  → products.						
82 ATK/ASC4 ¹⁾ 1) CH ₃ ONO/NO/2-Pentanone photolysis. [2-Pentanone] = (1.2-2.4)×10 ¹⁴ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-4.0)×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.	RN	299	(2.85±0.08)(12)			2
OH + (CH ₃ CH ₂) ₂ CO → products Hydroxyl + 3-Pentanone 82 ATK/ASC4 ¹⁾	RL	299	(2.45±0.44)(-1)			2/2
k _{ref} : OH +  → products.						
82 ATK/ASC4 ¹⁾ 1) CH ₃ ONO/NO/2-Pentanone photolysis. [3-Pentanone] = (1.2-2.4)×10 ¹⁴ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-4.0)×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.	RN	299	(1.11±0.20)(12)			2
OH + CH ₃ C(O)OCH ₂ CH ₂ CH ₃ → products Hydroxyl + Acetic acid propyl ester (n-Propyl nitrate) 77 WIN/LLO	RL	305	8.5(-2)			2/2
k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.						
77 WIN/LLO	RN	305	(2.6±0.5)(12)			2
OH + CH ₃ CH ₂ C(O)OCH ₂ CH ₃ → products Hydroxyl + Propanoic acid ethyl ester 78 CAM/PAR	EX	292	(1.06±0.15)(12)			2
Reaction of ester vapor with OH in Pyrex vessel with vacuum system. OH generated by the reaction of a H ₂ O ₂ /NO ₂ /CO mixture. P(Total) = 100 torr.						
OH + CH ₃ CH ₂ CH ₂ CH(CH ₃)ONO ₂ → products Hydroxyl + 2-Pentanol nitrate 82 ATK/ASC5 ¹⁾	RL	299	(2.47±0.16)(-1)			2/2
k _{ref} : OH +  → products.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 ATK/ASC5 ¹⁾ ¹⁾ CH ₃ ONO/NO/2-Pentanol nitrate photolysis. [CH ₃ ONO] ₀ = (0.9-7.1) × 10 ¹⁴ molec.cm ⁻³ . [Alkyl nitrate] = 2.4 × 10 ¹³ molec.cm ⁻³ .	RN	299	(1.13 ± 0.07)(12)			2
OH + (CH ₃ CH ₂) ₂ CHONO ₂ → products Hydroxyl + 3-Pentanol nitrate						
82 ATK/ASC5 ¹⁾	RL	299	(1.49 ± 0.26)(-1)			2/2
k _{ref} : OH +  → products.						
82 ATK/ASC5 ¹⁾ ¹⁾ CH ₃ ONO/NO/3-Pentanol nitrate photolysis. [CH ₃ ONO] ₀ = (0.9-7.1) × 10 ¹⁴ molec.cm ⁻³ . [Alkyl nitrate] = 2.4 × 10 ¹³ molec.cm ⁻³ .	RN	299	(6.81 ± 1.20)(11)			2
OH +  → products Hydroxyl + Cyclohexene						
76 DAR/WIN k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.	RL	305	1.53			2/2
76 DAR/WIN	RN	305	(4.7 ± 0.9)(13)			2
76 WU/JAP Cylindrical Pyrex Reactor. k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products. P = 760 torr.	RL	303	1.2			2/2
80 COX/DER1 HONO photosensitized oxidation in synthetic air. Gas-chromatography. Same data given in 80 COX. [NO] = [NO ₂] = (0.3-3.0) ppm. [HONO] = (3-20) ppm.	RN	298	3.73(13)			2
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH=CH ₂ → products Hydroxyl + 1-Hexene						
76 WU/JAP Cylindrical Pyrex Reactor. k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products. P = 760 torr.	RL	303	6.0(-1)			2/2
OH + (CH ₃) ₃ CCH=CH ₂ → products Hydroxyl + 1-Butene, 3,3-dimethyl-						
76 WU/JAP Cylindrical Pyrex Reactor. k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products. P = 760 torr.	RL	303	5.2(-1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + (CH₃)₂C=C(CH₃)₂ → products						
Hydroxyl + 2-Butene, 2,3-dimethyl-						
71 MOR/NIK2	RL	300	9.0			2/2
k _{ref} : OH + CH ₃ CH=CH ₂ → products.						
77 DAV ¹⁾	EX	298	(3.42±0.07)(13)			2
78 RAV/WAG ¹⁾	EX	298	(3.43±0.08)(13)			2
¹⁾ M = He. Flash-photolysis.						
Resonance-fluorescence. P(He) = 20 torr.						
82 ATK/ASC2 ²⁾	RL	299	(4.28±0.21)			2/2
k _{ref} : OH + CH ₃ CH=CH ₂ → products.						
82 ATK/ASC2 ²⁾	RN	299	(6.50±0.36)(13)			2
²⁾ CH ₃ ONO/NO/2,3-Dimethyl-2-butene/Propene photolysis.						
[(CH ₃) ₂ C=C(CH ₃) ₂] = (1.2-2.4)×10 ¹³ molec.cm ⁻³ .						
[CH ₃ ONO] ₀ = (9.5-3.5)×10 ¹⁴ molec.cm ⁻³ .						
P(Total) = 735 torr.						
OH +  → products						
Hydroxyl + Cyclohexane						
74 GOR/VOL	RL	298	4.48(1)			2/2
74 GOR/VOL	RN	298	(4.04±0.90)(12)			2
76 WU/JAP	RL	303	1.2(-1)			2/2
Cylindrical Pyrex Reactor.						
k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products.						
P = 760 torr.						
82 ATK/ASC2 ¹⁾	RL	299	(1.32±0.04)			2/2
k _{ref} : OH + CH ₃ (CH ₂)CH ₃ → products.						
82 ATK/ASC2 ¹⁾	RN	299	(4.53±0.16)			2
¹⁾ CH ₃ ONO/NO/Cyclohexane/Hexane photolysis.						
[Cyclohexane] = (1.2-2.4)×10 ¹³ molec.cm ⁻³ .						
[CH ₃ ONO] ₀ = (9.5-3.5)×10 ¹⁴ molec.cm ⁻³ .						
P(Total) = 735 torr.						
OH + CH₃(CH₂)₄CH₃ → H₂O + CH₃(CH₂)₄CH₂ (a)						
→ H₂O + CH₃(CH₂)₃CHCH₃ (b)						
→ H₂O + CH₃(CH₂)₂CH(CH₂)₂CH₃ (c)						
Hydroxyl + Hexane						
76 LLO/DAR2	RL	305	2.09			2/2
(k _a + k _b + k _c)/k _{ref} .						
k _{ref} : OH + CH ₃ CH ₂ CH ₂ CH ₃ → products.						
76 CAM/MCL ¹⁾	EX	292	(3.3±0.2)(12)			2
76 LLO/DAR2 ¹⁾	RN	305	(3.8±0.8)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 WU/JAP ¹⁾ Cylindrical Pyrex Reactor. k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products. P = 760 torr.	RL	303	1.1(-1)			2/2
82 ATK/ASC2 ¹⁾ CH ₃ ONO/NO/Hexane photolysis. [CH ₃ ONO] ₀ = (9.5-3.5) × 10 ¹⁴ molec.cm ⁻³ . [Hexane] = (1.2-2.4) × 10 ¹³ molec.cm ⁻³ . P(Total) = 735 torr.	EX	299	(3.43 ± 0.05)(12)			2
¹⁾ k _a + k _b + k _c .						
OH + (CH ₃) ₂ CHCH ₂ CH ₂ CH ₃ → H ₂ O + (CH ₃) ₂ CHCH ₂ CH ₂ CH ₂ (a)						
→ H ₂ O + (CH ₃) ₂ CHCH ₂ CH ₂ CH ₃ (b)						
→ H ₂ O + (CH ₃) ₂ CHCHCH ₂ CH ₃ (c)						
→ H ₂ O + (CH ₃) ₂ CCH ₂ CH ₂ CH ₃ (d)						
→ H ₂ O + CH ₂ CH(CH ₃)CH ₂ CH ₂ CH ₃ (e)						
Hydroxyl + Pentane, 2-methyl-						
76 LLO/DAR2 (k _a + k _b + k _c + k _d + k _e)/k _{ref} . k _{ref} : OH + CH ₃ CH ₂ CH ₂ CH ₃ → products.	RL	305	1.77			2/2
76 LLO/DAR2 ¹⁾	RN	305	(3.2 ± 0.6)(12)			2
80 COX/DER1 ¹⁾ HONO photosensitized oxidation in synthetic air. Gas-chromatography. [NO] = NO ₂ = (0.3-3.0) ppm. [HONO] = (3-20) ppm. Same data given in 80 COX.	RN	298	3.01(12)			2
¹⁾ k _a + k _b + k _c + k _d + k _e .						
OH + CH ₃ CH ₂ CH(CH ₃)CH ₂ CH ₃						
→ H ₂ O + CH ₃ CH ₂ CH(CH ₃)CH ₂ CH ₂ (a)						
→ H ₂ O + CH ₃ CH ₂ CH(CH ₃)CHCH ₃ (b)						
→ H ₂ O + CH ₃ CH ₂ C(CH ₃)CH ₂ CH ₃ (c)						
→ H ₂ O + CH ₃ CH ₂ CH(CH ₂)CH ₂ CH ₃ (d)						
→ H ₂ O + CH ₃ CHCH(CH ₃)CH ₂ CH ₃ (e)						
→ H ₂ O + CH ₂ CH ₂ CH(CH ₃)CH ₂ CH ₃ (f)						
Hydroxyl + Pentane, 3-methyl-						
76 LLO/DAR2 (k _a + k _b + k _c + k _d + k _e + k _f)/k _{ref} . k _{ref} : OH + CH ₃ CH ₂ CH ₂ CH ₃ → products.	RL	305	2.40			2/2
76 LLO/DAR2 k _a + k _b + k _c + k _d + k _e + k _f .	RN	305	(4.3 ± 0.9)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + (CH ₃) ₂ CHCH(CH ₃) ₂ → H ₂ O + CH ₂ CH(CH ₃)CH(CH ₃) ₂ (a) → H ₂ O + (CH ₃) ₂ CCH(CH ₃) ₂ (b)						
Hydroxyl + Butane, 2,3-dimethyl-						
78 DAR/ATK ¹⁾ k _a . Computed from an empirical formula.	CO	300	4.70(11)			2
78 DAR/ATK ¹⁾ k _b . Computed from an empirical formula.	CO	300	2.53(12)			2
¹⁾ Irradiation technique.						
76 DAR/WIN (k _a + k _b)/k _{ref} . k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.	RL	305	1.0(-1)			2/2
76 DAR/WIN k _a + k _b .	RN	305	(3.1±0.6)(12)			2
78 DAR/ATK k _a + k _b . Irradiation technique.	EX	300	(3.42±0.17)(12)			2
80 COX/DER1 k _a + k _b . HONO photosensitized oxidation in synthetic air. [NO] = [NO ₂] = (0.3-3.0) ppm. [HONO] = (3-20) ppm. Same data given in 80 COX.	RN	298	2.29(12)			2
82 ATK/ASC2 ²⁾ (k _a + k _b)/k _{ref} . k _{ref} : OH +  → products.	RL	299	(8.27±0.04)(-1)			2/2
82 ATK/ASC2 ²⁾ k _a + k _b .	RN	299	(3.77±0.04)(12)			2
²⁾ CH ₃ ONO/NO/2,3-Dimethylbutane/Cyclohexane photolysis. [CH ₃ ONO] ₀ = (9.5-3.5)×10 ¹⁴ molec.cm ⁻³ . [2,3-Dimethylbutane] = (1.2-2.4)×10 ¹³ molec.cm ⁻³ . P(Total) = 735 torr.						
OH + CH ₃ C(O)CH ₂ CH ₂ CH ₂ CH ₃ → products						
Hydroxyl + 2-Hexanone						
82 ATK/ASC4 ¹⁾ k _{ref} : OH +  → products.	RL	299	(1.21±0.08)			2/2
82 ATK/ASC4 ¹⁾	RN	299	(5.52±0.37)(12)			2
¹⁾ CH ₃ ONO/NO/2-Hexanone photolysis. [2-Hexanone] = (1.2-2.4)×10 ¹⁴ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-4.0)×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
OH + CH₃CH₂C(O)CH₂CH₂CH₃ → products							
Hydroxyl + 3-Hexanone							
82 ATK/ASC4 ¹⁾	RL	299	(9.19±0.38)(-1)				2/2
k _{ref} : OH +  → products.							
82 ATK/ASC4 ¹⁾	RN	299	(4.19±0.17)(12)				2
¹⁾ CH ₃ ONO/NO/3-Hexanone photolysis. torr. [3-Hexanone] = (1.3-2.4)×10 ¹⁴ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-4.0)×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.							
OH + CH₃C(O)CH₂CH(CH₃)₂ → products							
Hydroxyl + 2-Pentanone, 4-methyl-							
76 WIN/LLO	RL	305	3.0(-1)				2/2
k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.							
76 WIN/LLO	RN	305	(9.0±3.0)(12)				2
80 COX/DER1	RN	300	7.47(12)				2
HONO photosensitized oxidation in synthetic air. Gas-chromatography. [NO] = [NO ₂] = (0.3-3.0) ppm. [HONO] = (3-20) ppm. Same data given on 80 COX.							
81 COX/PAT	EX	296	(7.83±0.18)(12)				2
HONO/N ₂ /O ₂ /4-Methyl-2-pentanone photolysis. P = 760 torr.							
82 ATK/ASC4 ¹⁾	RL	299	(1.91±0.09)				2/2
k _{ref} : OH +  → products.							
82 ATK/ASC4 ¹⁾	RN	299	(8.73±0.42)(12)				2
¹⁾ CH ₃ ONO/NO/4-Methyl-2-Pentanone photolysis. [CH ₃ ONO] ₀ = (0.9-4.0)×10 ¹⁴ molec.cm ⁻³ . [4-Methyl-2-Pentanone] = (1.3-2.4)×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.							
OH + CH₃C(O)OCH(CH₃)CH₂CH₃ → products							
Hydroxyl + Acetic acid 1-methylpropyl ester (s-Butyl acetate)							
77 WIN/LLO	RL	305	1.1(-1)				2/2
k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.							
77 WIN/LLO	RN	305	(3.4±0.7)(12)				2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH₃CH₂CH₂OCH₂CH₂CH₃ → products						
Hydroxyl + Propane, 1,1'-oxybis- (di-n-Propyl ether)						
76 LLO/DAR1	RL	305	3.4(-1)			2/2
k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.						
76 LLO/DAR1	RN	305	(1.04±0.21)(13)			2
OH + CH₃CH₂CH₂CH₂CH(CH₃)ONO₂ → products						
Hydroxyl + 2-Hexanol nitrate						
82 ATK/ASC5 ¹⁾	RL	299	(4.22±0.20)(-1)			2/2
k _{ref} : OH +  → products.						
82 ATK/ASC5 ¹⁾	RN	299	(1.92±0.09)(12)			2
¹⁾ CH ₃ ONO/NO/2-Hexanol nitrate photolysis. [Alkyl nitrate] = 2.4×10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-7.1)×10 ¹⁴ molec.cm ⁻³ .						
OH + CH₃CH₂CH₂CH(CH₂CH₃)ONO₂ → products						
Hydroxyl + 3-Hexanol nitrate						
82 ATK/ASC5 ¹⁾	RL	299	(3.59±0.28)(-1)			2/2
k _{ref} : OH +  → products.						
82 ATK/ASC5 ¹⁾	RN	299	(1.64±0.13)(12)			2
¹⁾ CH ₃ ONO/NO/3-Hexanol nitrate photolysis. [Alkyl nitrate] = 2.4×10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-7.1)×10 ¹⁴ molec.cm ⁻³ .						
OH +  → products						
Hydroxyl + Cyclohexene, 1-methyl-						
76 DAR/WIN	RL	305	1.91			2/2
k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.						
76 DAR/WIN	RN	305	(5.8±1.2)(13)			2
OH + CH₃CH₂CH₂CH₂CH₂CH=CH₂ → products						
Hydroxyl + 1-Heptene						
76 DAR/WIN	RL	305	7.3(-1)			2/2
k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.						
76 DAR/WIN	RN	305	(2.2±0.5)(13)			2

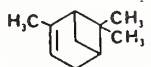
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH ₃ (CH ₂) ₅ CH ₃ → H ₂ O + CH ₃ (CH ₂) ₅ CH ₂ (a)						
→ H ₂ O + CH ₃ (CH ₂) ₄ CHCH ₃ (b)						
→ H ₂ O + CH ₃ (CH ₂) ₃ CHCH ₂ CH ₃ (c)						
→ H ₂ O + CH ₃ (CH ₂) ₂ CH(CH ₂) ₂ CH ₃ (d)						
Hydroxyl + Heptane						
82 ATK/ASC3 ¹⁾ (k _a + k _b + k _c + k _d)/k _{ref} . k _{ref} : OH + CH ₃ (CH ₂) ₄ CH ₃ → products.	RL	299	(1.28±0.02)			2/2
82 ATK/ASC3 ¹⁾ k _a + k _b + k _c + k _d .	RN	299	(4.40±0.10)(12)			2
¹⁾ CH ₃ ONO/NO/Heptane photolysis. [Heptane] = (1.2-2.4)×10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (2.1-4.0)×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.						
OH + (CH ₃) ₃ CCH(CH ₃) ₂ → H ₂ O + CH ₂ C(CH ₃) ₂ CH(CH ₃) ₂ (a)						
→ H ₂ O + (CH ₃) ₃ CCH(CH ₃)CH ₂ (b)						
→ H ₂ O + (CH ₃) ₃ CC(CH ₃) ₂ (c)						
Hydroxyl + Butane, 2,2,3-trimethyl-						
81 BAL/WAL2 (k _a + k _b)/k _{ref} . k _{ref} : OH + H ₂ → H ₂ O + H. Estimated ratio. Oxidation of 2,2,3-Trimethylbutane in H ₂ /O ₂ , in aged boric-acid-coated reaction vessels. P(2,2,3-Trimethylbutane) = 5 torr. P(Total) = 500 torr.	RL	753	6.7			2/2
76 DAR/WIN (k _a + k _b + k _c)/k _{ref} . k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.	RL	305	7.4(-2)			2/2
76 DAR/WIN k _a + k _b + k _c .	RN	305	(2.3±0.5)(12)			2
81 BAL/WAL2 ¹⁾ (k _a + k _b + k _c)/k _{ref} . Optimization. k _{ref} : OH + H ₂ → H ₂ O + H.	RL	300-500	(1.22±0.15)(1)	0	0	2/2
81 BAL/WAL2 ¹⁾ k _a + k _b + k _c .	SE	300-500	(5.92±0.50)(12)	0	217±42	2
81 BAL/WAL2 ¹⁾ k _c /k _{ref} . k _{ref} : OH + H ₂ → H ₂ O + H. Estimated ratio.	RL	753	5.5			2/2
81 BAL/WAL2 ¹⁾ k _c .	ES	300-1500	1.70(12)	0	-115±96	2 1.23
¹⁾ Oxidation of 2,2,3-Trimethylbutane in H ₂ O ₂ mixtures, in aged boric-acid-coated reaction vessels. Gas-chromatography. P(Total) = 500 torr. P(2,2,3-Trimethylbutane) = 5 torr.						

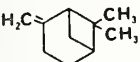
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + (CH ₃) ₂ CHC(O)CH(CH ₃) ₂ → products Hydroxyl + 3-Pentanone, 2,4-dimethyl- 82 ATK/ASC4 ¹)	RL	299	(7.17±0.54)(-1)			2/2
k _{ref} : OH +  → products. 82 ATK/ASC4 ¹)	RN	299	(3.27±0.24)(12)			2
1) CH ₃ ONO/NO/2,4-Dimethyl-3-Pentanone photolysis. [2,4-Dimethyl-3-Pentanone] = (1.3-2.4)×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr. [CH ₃ ONO] ₀ = (0.9-4.0)×10 ¹⁴ molec.cm ⁻³ .						
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH(CH ₂ CH ₃)ONO ₂ → products Hydroxyl + 3-Heptanol nitrate 82 ATK/ASC5 ¹)	RL	299	(4.91±0.57)(-1)			2/2
k _{ref} : OH +  → products. 82 ATK/ASC5 ¹)	RN	299	(2.24±0.26)(12)			2
1) CH ₃ ONO/NO/3-Heptanol nitrate photolysis. [Alkyl nitrate] = 2.4×10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-7.1)×10 ¹⁴ molec.cm ⁻³ .						
OH + CH ₃ (CH ₂) ₆ CH ₃ → H ₂ O + CH ₃ (CH ₂) ₆ CH ₂ (a) → H ₂ O + CH ₃ (CH ₂) ₅ CHCH ₃ (b) → H ₂ O + CH ₃ (CH ₂) ₄ CHCH ₂ CH ₃ (c) → H ₂ O + CH ₃ (CH ₂) ₃ CH(CH ₂) ₂ CH ₃ (d) Hydroxyl + Octane 82 ATK/ASC3 ¹)	RL	299	(1.58±0.02)			2/2
(k _a + k _b + k _c + k _d)/k _{ref} . k _{ref} : OH + CH ₃ (CH ₂) ₄ CH ₃ → products. 82 ATK/ASC3 ¹)	RN	299	(5.43±0.11)(12)			2
k _a + k _b + k _c + k _d . 1) CH ₃ ONO/NO/Octane photolysis. [Octane] = (1.2-2.4)×10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (2.1-4.0)×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.						
OH + CH ₃ (CH ₂) ₄ CH(CH ₂ CH ₃)ONO ₂ → products Hydroxyl + 3-Octanol nitrate 82 ATK/ASC5 ¹)	RL	299	(5.16±1.05)(-1)			2/2
k _{ref} : OH +  → products.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/(ref), A, A/(ref)	n	B, B-B(ref)	k, A k err. units factor
82 ATK/ASC5 ¹⁾ 1) CH ₃ ONO/NO/3-Octanol nitrate photolysis. [Alkyl nitrate] = 2.4x10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-7.1)x10 ¹⁴ molec.cm ⁻³ .	RN	299	(2.35±0.48)(12)			2
OH + CH ₃ (CH ₂) ₇ CH ₃ → H ₂ O + CH ₃ (CH ₂) ₇ CH ₂ (a) → H ₂ O + CH ₃ (CH ₂) ₆ CHCH ₃ (b) → H ₂ O + CH ₃ (CH ₂) ₅ CHCH ₂ CH ₃ (c) → H ₂ O + CH ₃ (CH ₂) ₄ CH(CH ₂) ₂ CH ₃ (d) → H ₂ O + CH ₃ (CH ₂) ₃ CH(CH ₂) ₃ CH ₃ (e)						
Hydroxyl + Nonane						
82 ATK/ASC3 ¹⁾ (k _a + k _b + k _c + k _d + k _e)/k _{ref} . k _{ref} : OH + CH ₃ (CH ₂) ₄ CH ₃ → products.	RL	299	(1.87±0.05)			2/2
82 ATK/ASC3 ¹⁾ k _a + k _b + k _c + k _d + k _e . 1) CH ₃ ONO/NO/Nonane photolysis. [Nonane] = (1.2-2.4)x10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (2.1-4.0)x10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.	RN	299	(6.44±0.24)(12)			2
OH + (CH ₃) ₂ CHCH ₂ COCHCH ₂ (CH ₃) ₂ → products						
Hydroxyl + 4-Heptanone, 2,6-dimethyl-						
76 WIN/LLO k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.	RL	305	5.0(-1)			2/2
76 WIN/LLO	RN	305	(1.5±0.5)(13)			2
82 ATK/ASC4 ¹⁾ k _{ref} : OH +  → products.	RL	299	(3.66±0.19)			2/2
82 ATK/ASC4 ¹⁾ 1) CH ₃ ONO/NO/2,6-Dimethyl-4-Heptanone photolysis. [2,6-Dimethyl-4-Hexanone] = (1.3-2.4)x10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr. [CH ₃ ONO] ₀ = (0.9-4.0)x10 ¹⁴ molec.cm ⁻³ .	RN	299	(1.67±0.09)(12)			2
OH +  → products						
Hydroxyl + Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl- (α-Pinene)						
82 KLE/HAR OH generated by H ₂ O flash-photolysis. Resonance-fluorescence. P(Total) = 50 torr. (Ar)	EX	297-424	8.25(12)	0	-446±75	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH +  → products						
Hydroxyl + Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene- (β -Pinene)						
82 KLE/HAR OH generated by the H ₂ O flash-photolysis. Resonance-fluorescence. P(Total) = 50 torr. (Ar)	EX	297-424	1.42(13)	0	-358±58	2
OH + CH ₃ (CH ₂) ₈ CH ₃ → H ₂ O + CH ₃ (CH ₂) ₈ CH ₂ (a) → H ₂ O + CH ₃ (CH ₂) ₇ CHCH ₃ (b) → H ₂ O + CH ₃ (CH ₂) ₆ CHCH ₂ CH ₃ (c) → H ₂ O + CH ₃ (CH ₂) ₅ CH(CH ₂) ₂ CH ₃ (d) → H ₂ O + CH ₃ (CH ₂) ₄ CH(CH ₂) ₃ CH ₃ (e)						
Hydroxyl + Decane						
82 ATK/ASC3 1) (k _a + k _b + k _c + k _d + k _e)/k _{ref} . k _{ref} : OH + CH ₃ (CH ₂) ₄ CH ₃ → products.	RL	299	(2.00±0.09)			2/2
82 ATK/ASC3 1) k _a + k _b + k _c + k _d + k _e . 1) CH ₃ ONO/NO/Decane photolysis. P(Total) = 735 torr. [CH ₃ ONO] ₀ = (2.1-4.0)×10 ¹⁴ molec.cm ⁻³ . [Decane] = (1.2-2.4)×10 ¹³ molec.cm ⁻³ .	RN	299	(6.87±0.36)(12)			2
HO ₂ + O ₃ → OH + O ₂ + O ₂						
Hydroperoxo + Ozone						
73 AND/KAU2 Upper-limit k.	EX	220-450	≤3.01(9)			2
73 DEM	EX	300	1.81(9)			2
73 SIM/HEI3	RN	225-298	1.98(10)	0	1007	2
74 DEM/TSC	ES	273-342	1.20(11)	0	1560±252	2 2.0
79 SU/CAL1 Cl ₂ /O ₃ /H ₂ photolysis in O ₂ /N ₂ . FTIR-, and IR-Spectroscopy. Upper-limit k. P(Total) = 700 torr.	ES	298	≤(1.33±0.66)(9)			2
80 ZAH/HOW Discharge-flow. Laser magnetic resonance.	EX	245-365	(8.43±2.41)(9)	0	580±100	2
HO ₂ + HO ₂ (+ M) → H ₂ O ₂ + O ₂ (+ M)						
Hydroperoxo						
72 HOC/GHO	EX	298	(5.7±0.5)(12)			2
72 PAU/JOH	EX	295	(2.17±0.30)(12)			2
75 HAM	EX	298	1.90(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 HAM/LII 1)	EX	298	1.51(12)			2	1.20
77 HAM/LII 1)	RL	298	2.83			2/2	
k _{ref} : DO ₂ + DO ₂ → H ₂ O ₂ + O ₂ .							
77 HAM/LII 1)	EX	298	1.51(12)			2	
1) Electron pulse radiolysis and Kinetic Spectrometry.							
P(H ₂) = 2 atm. P(O ₂) = 5 torr.							
78 COX 2)	EX	273	2.05(12)			2	
78 COX 2)	EX	298	(1.39±0.18)(12)			2	
78 COX 2)	EX	338	9.03(11)			2	
2) Cl ₂ /H ₂ /NO ₂ photolysis in N ₂ /O ₂ . P = 1 atm.							
79 BUR/CLI	EX	298	≤7.23(11)			2	
Discharge-flow. Upper-limit k.							
79 COX/BUR	EX	273-339	(2.29±0.84)(10)	0	-1250±200	2	
UV-Absorption spectrometry. P = (3-760) torr.							
k dependent on P(H ₂ O) and increasing with T.							
Negative values of E _a and pressure effects discussed in terms of a complex forming mechanism.							
79 GRA/WIN	EX	300	2.29(12)			2	2.0
Thermolysis of HO ₂ NO ₂ .							
P(Total) = 760 torr.							
79 LII/GOR	EX	276-400	(6.87±0.96)(10)	0	-1057±45	2	
Pulse-radiolysis. Kinetic Spectrophotometry.							
79 THR/WIL 3)	EX	298	(1.75±0.72)(11)			2	
P(He) = 2 torr.							
79 THR/WIL 3)	EX	298	(2.59±1.08)(11)			2	
P(He) = 3 torr.							
79 THR/WIL 3)	EX	298	(3.31±0.84)(11)			2	
P(He) = 4 torr.							
79 THR/WIL 3)	EX	298	(4.46±1.99)(11)			2	
P(Ar) = 2.2 torr.							
3) Laser magnetic-resonance spectroscopy in a flow-reactor.							
80 HOC/SWO2	EX	296	(4.0±0.7)(12)			2	
H ₂ O flash-photolysis in presence of O ₂ and CO (or He). P = 760 torr.							
80 LII/GOR1 4)	ES	290-400	(5.36±0.18)(10)	0	-1057	2	
80 LII/GOR1 4)	ES	298	1.87(12)			2	
4) Electron pulse-radiolysis.							
Kinetic spectrophotometry.							
P(Total) = 1200 torr.							
81 BUR/COX 5)	EX	308	(1.25±0.12)(12)			2	
P(H ₂ O) = 0							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 BUR/COX ⁵) P(H ₂ O) = 3.0 torr.	EX	308	(1.33±0.12)(12)			2
81 BUR/COX ⁵) P(H ₂ O) = 0	EX	348	(8.07±0.90)(11)			2
81 BUR/COX ⁵) P(H ₂ O) = 10.5 torr.	EX	348	(9.52±0.90)(11)			2
⁵) O ₃ /H ₂ O/O ₂ /N ₂ (or He) photolysis. Molecular Modulation. P(Total) = 760 torr.						
81 LII/SAU Pulse-radiolysis. k estimated in terms of a complex-forming mechanism.	ES	298-373	(5.54±0.12)(10)	0	-1057	2
82 PAT/PIL HO ₂ generated by the CH ₃ OH/O ₂ /Cl ₂ flash- photolysis in N ₂ . P(CH ₃ OH) ~ P(Cl ₂) ~ 1.5 torr. P(Total) = 700 torr. P(O ₂) ~ 5 torr.	EX	298-510	(2.49±0.69)(11)	0	-630±115	2
82 SAN/PET ⁶) HO ₂ generated by the Cl ₂ /CH ₃ OH/O ₂ photolysis.	EX	298	(9.64±1.20)(11)			2
82 SAN/PET ⁶) HO ₂ generated by the Cl ₂ /H ₂ /O ₂ photolysis. P(H ₂) = 130 torr. P(O ₂) = 560 torr.	EX	298	(1.54±0.11)(12)			2
⁶) Flash-photolysis. UV-absorption spectrometry.						
82 SIM/HEI ⁷) Limiting low-pressure k.	EX	296	(8.43±1.20)(11)			2
82 SIM/HEI ⁷) P(N ₂) = 760 torr.	EX	296	(1.51±0.06)(12)			2
⁷) Flash-photolysis. UV-absorption spectrometry. HO ₂ generated by the Cl ₂ /CH ₃ OH/O ₂ photolysis. M = He, or N ₂ . P-dependent from 5 to 770 torr. [HO ₂] = (1.3-3.3)×10 ¹⁴ molec.cm ⁻³ .						
82 THR/TYN2 Flash-photolysis combined with tunable-diode La- ser-spectroscopy. HO ₂ generated the Cl ₂ /CH ₃ OH/O ₂ photolysis. k is P-independent within the given range. [HO ₂] ₀ = (0.58-1.20)×10 ¹⁵ molec.cm ⁻³ . P(Total) = (7-20) torr.	EX	298-358	1.44(11)	0	-560	2
82 SAN/PET M = He. M-efficiencies relative to He are: 1.0(He), 1.61(Ar), 1.67(O ₂), 1.33(N ₂), 2.75(SF ₆). Flash-photolysis. UV-Absorption-spectroscopy. HO ₂ generated by photolysing Cl ₂ /CH ₃ OH/O ₂ . Limiting low-pressure k's within the (100-700) torr. range.	EX	298	8.34(15)			3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
DO₂ + DO₂ → D₂O₂ + O₂						
Hydroperoxo-d ₂						
77 HAM/LII	EX	298	5.32(11)			2 1.20
77 HAM/LII	EX	298	5.32(12)			2
Electro-n pulse radiolysis. Kinetic spectro- photometry. P(H ₂) = 2 atm. P(O ₂) = 5 torr.						
82 SAN/PET	EX	298	(4.22±0.24)(11)			2
HO ₂ generated by the Cl ₂ /D ₂ /O ₂ flash-photolysis. UV-absorption spectrometry. P = 700 torr.						
HO₂ + SO₂ (+ M) → OH + SO₃ (+ M) (a)						
→ HO ₂ SO ₂ (+ M) (b)						
Hydroperoxo + Sulfur dioxide						
73 PAY/STI ¹⁾	RN	300	(5.24±0.18)(8)			2
79 BUR/CLI ¹⁾	EX	298	≤1.20(7)			2
Discharge-flow. Upper-limit k.						
79 GRA/WIN ¹⁾	EX	300	≤6.02(5)			2
HO ₂ NO ₂ thermolysis. Upper-limit k. P(Total) = 760 torr.						
¹⁾ k _a .						
79 BUR/CLI	EX	298	≤1.45(14)			3
k _b . M = He. Discharge-flow. Upper-limit k.						
HO₂ + NO (+ M) → O₂ + HNO (+ M) (a)						
→ OH + NO ₂ (+ M) (b)						
→ HONO ₂ (+ M) (c)						
Hydroperoxo + Nitrogen oxide (NO)						
79 HOW ¹⁾	EX	271	<1.81(10)			2
79 HOW ¹⁾	EX	303	<6.02(9)			2
¹⁾ k _a . Upper-limit k's. Discharge-flow. Laser-Magnetic Resonance.						
74 SIM/HEI2	RL	298	(7.0±1.0)			2/2
k _b /k _{ref} . k _{ref} : HO ₂ + NO ₂ → HONO + O ₂						
73 PAY/STI ²⁾	ES	300	1.8(11)			2 3.0
73 SIM/HEI1 ²⁾	ES	298	>9.03(10)			2
Lower-limit k.						
74 HAC/HOY2 ²⁾	EX	298-669	(2.0±1.0)(13)	0	1430	2
75 COX ²⁾	ES	300	(7.23±1.81)(11)			2
75 COX/DER1 ²⁾	ES	296	(7.23±1.81)(11)			2
75 GLA/TRO ²⁾	ES	1350-1700	(4.5±1.0)(12)			2
75 HAC/HOY ²⁾	EX	298-670	(1.2±0.3)(13)	0	1200±150	2
76 SIM/HEI ²⁾	RN	296	(6.02±1.20)(11)			2 1.2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
77 HOW/EVE ³⁾	EX	296	(4.88±0.90)(12)			2
77 SIM/HEI ³⁾	ES	245-328	7.23(12)	0	705±252	2
78 COX ³⁾	ES	283	2.47(12)			2
Cl ₂ /H ₂ /NO ₂ photolysis in molar N ₂ /O ₂ . P = 1 atm.						
78 MAR/AND ³⁾	EX	298	(4.22±1.81)(12)			2
Discharge-flow. Resonance-fluorescence.						
Unreported T assumed to be 298 K.						
78 PRE ³⁾	EX	293	(2.4±0.7)(12)			2
Laser Magnetic Resonance Spectrometry.						
78 SIM/HEI ³⁾	RN	245-328	7.23(12)	0	705±252	2
Determined relative to the reaction:						
HO ₂ + HO ₂ → H ₂ O ₂ + O ₂ .						
N ₂ O/H ₂ /O ₂ /NO Photolysis.						
79 BUR/CLI ³⁾	EX	298	(4.94±1.45)(12)			2
Conventional discharge-flow system.						
79 HOW ³⁾	EX	232-403	(1.99±0.42)(12)	0	-254±50	2
n = 0 assumed. Discharge-flow. Magnetic-Resonance.						
79 HOW ³⁾	EX	232-403	(4.79±0.61)(12)	-0.83	0	2
Discharge-flow. Magnetic-Resonance.						
The preexponential factor expressed as: A(T/298) ^{-0.83} .						
79 LEU ³⁾	EX	270-425	(3.43±3.37)(12)	0	-130±270	2
Discharge-flow. Resonance-fluorescence.						
80 GLA/LEI ³⁾	EX	297	(6.63±1.81)(12)			2
Discharge-flow. Same data given in 79 GLA/LEI.						
80 HAC/PRE ³⁾	EX	293	(4.6±1.0)(12)			2
Isothermal discharge-flow. ESR-LMR Spectrometry.						
80 HOW ³⁾	EX	232-1271	(2.11±0.21)(12)	0	-240±30	2
Discharge-flow. Laser Magnetic Resonance.						
80 LOR/AZA ³⁾	EX	873	9.64(11)			2
H ₂ /O ₂ combustion in presence of Propane and NO.						
81 THR/WIL ³⁾	EX	298	(4.16±0.36)(12)			2
Laser magnetic resonance spectrometry.						
³⁾ k _b .						
76 SIM/HEI	RL	295	(9.5±1.5)			2/2
(k _b + k _c)/k _{ref} . Estimated ratio.						
k _{ref} : HO ₂ + NO ₂ → [HO ₂ NO ₂].						
78 SIM/HEI	RL	245-328	(1.7±0.4)	0	0	2/2
(k _b + k _c)/k _{ref} . k _{ref} : HO ₂ + NO ₂ → HONO + O ₂ (d)						
→ HO ₂ NO ₂ (e)						
T-independent rate ratio assumed.						
N ₂ O/H ₂ /O ₂ /NO Photolysis.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 COX/DER1 ⁴⁾	ES	296	(8.43±2.11)(10)			2
76 SIM/HEI ⁴⁾	RN	296	<1.20(9)			2
Upper-limit k.						
78 SIM/HEI ⁴⁾	ES	245	≈(1.2±0.6)(10)			2
N ₂ O/H ₂ /O ₂ /NO photolysis.						
⁴⁾ k _c .						
78 SIM/HEI	RL	245	(3.0±1.0)(-1)			2/2
N ₂ O/H ₂ /O ₂ /NO photolysis.						
k _c /(k _b + k _c).						
79 HOW ⁵⁾	EX	271	<1.45(17)			3
79 HOW ⁵⁾	EX	303	<4.72(16)			3
⁵⁾ k _c . M = He + O ₂ . Upper-limit k's.						
Discharge-flow.						
DO ₂ + NO → OD + NO ₂						
Hydroperoxo-d + Nitrogen oxide (NO)						
80 GLA/LEI	EX	297	(6.63±2.11)(12)			2
Discharge-flow. Same data given in 79 GLA/LEI.						
HO ₂ + NO ₂ (+ M) → HONO + O ₂ (+ M) (a)						
→ HO ₂ NO ₂ (+ M) (b)						
Hydroperoxo + Nitrogen oxide (NO ₂)						
75 GLA/TRO ¹⁾	RL	1350-1700	(2.2±0.8)(-1)			2/2
Estimated ratio. k _{ref} : HO ₂ + NO → HO + NO ₂ .						
77 LEV/USE ¹⁾	RL	297	(4.3±2.0)(-2)			2/2
Estimated ratio. k _{ref} : HO ₂ + NO → OH + NO ₂ .						
78 SIM/HEI ¹⁾	RL	245	<8.7(-3)			2/2
Upper-limit ratio. N ₂ O/H ₂ /O ₂ /NO photolysis.						
k _{ref} : HO ₂ + NO → OH + NO ₂ (a)						
→ HONO ₂ (b)						
¹⁾ k _a /k _{ref} .						
77 LEV/USE	RL	297	(7.0±0.4)(-1)			2/2
k _a /k _b . Estimated ratio.						
74 SIM/HEI ²⁾	ES	298	>1.81(11)			2
Lower-limit k.						
75 COX ²⁾	RN	300	(7.23±1.81)(10)			2
75 COX/DER1 ²⁾	ES	296	(7.23±1.81)(10)			2
77 HOW ²⁾	EX	300	<1.81(9)			2
Upper-limit k.						
80 LIT ²⁾	EX	263	<3.01(10)			2
Conventional IR Absorption Spectroscopy.						
P = 30 torr. Upper-limit k.						
²⁾ k _a .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
76 SIM/HEI k _a + k _b .	ES	296	(1.18±0.42)(11)			2	
77 COX/DER ³⁾ HONO Photolysis in presence of CO. k _{ref} : HO ₂ + NO → OH + NO ₂	RL	273-328	(2.2±0.3)			2/2	
77 LEV/USE ³⁾ k _{ref} : HO ₂ + NO → OH + NO ₂ . Estimated ratio.	RL	297	(5.8±2.0)(-2)			2/2	
77 SIM/HEI ³⁾ k _{ref} : HO ₂ + NO → OH + NO ₂ .	RL	245	(6.1±1.5)(-1)			2/2	
78 SIM/HEI ³⁾ N ₂ O/H ₂ /O ₂ /NO photolysis. Estimated ratio. k _{ref} : HO ₂ + NO → OH + NO ₂ (a) → HONO ₂ (b)	RL	245	(6.1±1.5)(-1)			2/2	
³⁾ k _b /k _{ref} .							
76 SIM/HEI ⁴⁾	ES	296	(5.90±2.10)(10)			2	
77 SIM/HEI ⁴⁾	ES	245-328	2.53(11)	0	0	2	
78 COX ⁴⁾ High-pressure k, estimated by extrapolation experimental data. Cl ₂ /H ₂ /NO ₂ photolysis in equimolar N ₂ /O ₂ at P = 1 atm.	ES	283	5.42(11)			2	
78 SIM/HEI ⁴⁾ N ₂ O/H ₂ /O ₂ /NO photolysis. T-independent k.	EX	245-328	2.53(11)	0	0	2	
79 COX/PAT ⁴⁾ Limiting high-pressure k. Molecular modulation-UV Absorption spectrometry.	EX	283	(9.03±3.01)(11)			2	
81 MOR/HEI ⁴⁾ Photolysis of NO ₂ in presence of HCHO and O ₂ , at 360 nm. M = O ₂ (54 torr.) + HCHO(2 torr.)	EX	296	4.22(11)			2	2.0
77 HOW ⁴⁾ M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.47(He), 0.72(O ₂), 3.16(NO ₂).	EX	300	(7.58±1.89)(16)			3	
78 COX ⁴⁾ M = N ₂ + O ₂ . Low-pressure k, determined on the basis of a simple Lindemann-Hinshelwood model. Cl ₂ /H ₂ /NO ₂ photolysis in equimolar N ₂ /O ₂ . P = 1 atm.	EX	338	(9.07±1.09)(16)			3	
79 COX/PAT ⁴⁾ Limiting low-pressure k. M = N ₂ + O ₂ . Molecular modulation-UV Absorption Spectrometry.	EX	283	(9.07±1.81)(16)			3	
⁴⁾ k _b .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
$\text{HO}_2 + \text{N}_2\text{O} \rightarrow \text{OH} + \text{N}_2 + \text{O}_2$ (a) → any other products (b) Hydroperoxo + Nitrogen oxide (N_2O)						
79 HOW k _a . Discharge-flow system. Laser Magnetic Resonance. Upper-limit k.	EX	300-394	<3.01(6)			2
79 GRA/WIN k _{overall} . Thermolysis of HO_2NO_2 . Upper-limit k. P(Total) = 760 torr.	EX	300	≤1.20(4)			2
79 HOW k _{overall} . Discharge-flow system. Laser Magnetic Resonance. Upper-limit k.	EX	300-394	≤3.0(7)			2
$\text{HO}_2 + \text{NH}_2 \rightarrow \text{NH}_3 + \text{O}_2$ (a) → $\text{H}_2\text{O} + \text{HNO}$ (b) Hydroperoxo + Amidogen						
79 CHE/SAR k _a + k _b . NH_3 flash-photolysis. Laser Spectroscopy. P = (100-570) torr.	EX	298	(1.51±0.30)(13)			2
79 LOZ/NAD k _a + k _b . Intracavity Laser Spectroscopy. Flash-photolysis. P = (10-760) torr.	RN	298	(3.67±1.51)(13)			2
79 NAD/SAR1 k _b /(k _a + k _b). NH_3/O_2 Pulse-photolysis. Intracavity Laser Spectroscopy. Lower-limit ratio.	RL	298	≥3.0(-1)			2/2
$\text{HO}_2 + \text{CO} (+ \text{M}) \rightarrow \text{OH} + \text{CO}_2 (+ \text{M})$ Hydroperoxo + Carbon monoxide						
72 VAR/DAN	EX	878-952	1.33(14)	0	11575±1510	2
72 WES/DEH1 k _{ref} : $\text{HO}_2 + \text{H} \rightarrow \text{OH} + \text{OH}$. Estimated ratio.	RL	298	(6.0±2.0)(-2)			2/2
73 GOR Upper-limit k.	EX	298	<9.6(7)			2
73 DAV/PAY Estimated, upper-limit k.	ES	300	≤6.02(3)			2
73 SIM/HEI1 Estimated, upper-limit k.	ES	373-473	<3.01(6)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
74 WYR/WEN Upper limit k derived from spectroscopic observations.	EX	310	$\leq 1.6(10)$			2
74 WYR/WEN Upper limit k derived from CO ₂ yield measurements.	EX	310	$\leq 2.0(6)$			2
75 VAR/SAC	EX	878-952	$(1.07 \pm 0.30)(14)$	0	11575 $\pm$ 1510	2
77 ATR/BAL P(Total) = 500 torr. Determined relative to the reaction: $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$.	RN	~773	5.8(13)	0	11547	2
77 COL/NAE	ES	1110	5.6(9)			2 4.0
79 BUR/CLI Discharge-flow. Upper-limit k.	EX	298	$\leq 1.20(7)$			2
79 GRA/WIN Thermolysis of HO ₂ NO ₂ . Upper-limit k. P(Total) = 760 torr.	EX	300	$\leq 1.20(5)$			2
79 HOW ¹⁾	EX	304	$< 2.41(7)$			2
79 HOW ¹⁾	EX	394	$< 3.61(9)$			2
¹⁾ Discharge-flow. Upper-limit k's.						
79 BUR/CLI M = He. Discharge-flow. Upper-limit k.	EX	298	$\leq 1.45(14)$			3
$\text{HO}_2 + \text{CH}_4 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3$ Hydroperoxo + Methane						
72 SKI/LIF	ES	1000-2500	2.0(13)	0	9059	2
$\text{HO}_2 + \text{HCHO} \rightarrow \text{O}_2 + \text{CH}_2\text{OH}$ (a) $\rightarrow \text{H}_2\text{O}_2 + \text{CHO}$ (b) $\rightarrow \text{HO}_2\text{CH}_2\text{O} \rightarrow \text{HOCH}_2\text{O}_2$ (c) Hydroperoxo + Formaldehyde						
81 TSU/HAS k_a . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ in Ar behind reflected shock-waves. $k_1 = k_{-1}K$.	DE	1200-1800	3.39(12)	0	9623	2
71 BAL/LAN ¹⁾	ES	713	1.36(9)			2
71 BAL/LAN ¹⁾	ES	673-773	1.0(12)	0	5033 $\pm$ 1007	2
72 BAL/FUL ¹⁾	DE	673-773	9.6(8)			2
71 VAR/SAC ¹⁾ Oxidation in quartz reactor.	EX	773-973	1.14(13)	0	5234 $\pm$ 1510	2
¹⁾ k_b .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 SU/CAL3 k_c . Photolysis of Cl_2/HCHO mixtures diluted in synthetic air. FTIR Spectroscopy. P(Total) ~ 700 torr.	ES	298	~6.02(9)			2
82 VEY/RAY k_c . $\text{HCHO}/\text{O}_2/\text{NO}$ flash-photolysis. Data-fit by computer simulation on the basis of a proposed mechanism. [NO] ₀ = (15-200) torr. [O ₂] ₀ = (2.5-45) torr. [HCHO] ₀ = (2-30) torr.	DE	298	(4.52±2.11)(10)			2
$\text{HO}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{O}_2 + \text{CH}_3\text{OOH}$						
Hydroperoxo + Methylidioxo						
79 COX/TYN ¹⁾	EX	274	(5.12±0.72)(12)			2
79 COX/TYN ¹⁾	EX	298	(3.61±0.54)(12)			2
79 COX/TYN ¹⁾	EX	338	(2.11±0.30)(12)			2
80 COX/TYN ¹⁾ P = 760 torr.	EX	275-338	4.63(10)	0	-1296±364	2 3.4
¹⁾ Molecular Modulation UV-Absorption Spectrometry.						
$\text{HO}_2 + \text{CH}_3\text{OH} \rightarrow \text{H}_2\text{O}_2 + \text{CH}_2\text{OH}$						
Hydroperoxo + Methanol						
81 TSU/HAS M = Ar. Thermal oxidation of $\text{CH}_3\text{OH}/\text{O}_2$ mixtures mixtures diluted in Ar, behind reflected shock-waves.	ES	1200-1800	1.0(12)	0	5052	2
$\text{HO}_2 + \text{CH}_2=\text{CH}_2 \rightarrow \text{OH} + \text{C}_2\text{H}_3\text{O}$						
Hydroperoxo + Ethene						
73 WAL2 k_{ref} :	RL	773	(1.6±0.2)(-2)			2/2
$\text{HO}_2 + \text{HCHO} \rightarrow \text{H}_2\text{O}_2 + \text{CHO}$						
73 WAL2	ES	773	1.5(7)			2
81 BAL/WAL1 Oxidation of Ethene in H_2/O_2 mixtures in aged boric-acid-coated vessels.	ES	773	(5.0±1.0)(7)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
HO₂ + CH₃CH₃ → H₂O₂ + CH₃CH₂							
Hydroperoxo + Ethane							
71 BAL/LAN k _{ref} : CH ₃ CH ₃ + HCHO → products. Estimated ratio.	RL	713	2.8(-2)			2/2	
73 BAL/FUL k _{ref} : HO ₂ + HCHO → H ₂ O ₂ + CHO. Rate ratio per primary C-H bond: k _{prim} /k _{ref} = 0.005	RL	773	3.0(-2)			2/2	
73 BAL/FUL Rate constant per primary C-H bond: k _{prim} = 5.1x10 ⁶ cm ³ mol ⁻¹ s ⁻¹	RN	773	3.06(7)			2	
HO₂ + CH₃CHO → H₂O₂ + CH₃CO							
Hydroperoxo + Acetaldehyde							
77 COL/NAE	ES	1030-1115	1.70(12)	0	5350	2	4.0
HO₂ + CH₂CH₂OH → O₂ + CH₃CH₂OH (a) → H₂O + HCHO + HCHO (b)							
Hydroperoxo + Ethyl, 2-hydroxy-							
76 MEA/HEI k _a /k _b .	RL	298	1.2			2/2	
HO₂ + CH₃CH=CH₂ → OH + 							
Hydroperoxo + 1-Propene							
77 SAR/VAR Oxidation of Formaldehyde in presence of Propane. Upper-limit k.	ES	823	≤1.08(8)			2	
81 BAL/WAL1 Oxidation of 1-Propene in H ₂ /O ₂ mixtures, in aged boric-acid- coated vessels.	ES	773	1.5(8)			2	
HO₂ + CH₃CH₂CH₃ → H₂O₂ + (CH₃)₂CH (a) → H₂O₂ + CH₃CH₂CH₂ (b)							
Hydroperoxo + Propane							
71 BAL/LAN (k _a + k _b)/k _{ref} . k _{ref} : HCHO + CH ₃ CH ₂ CH ₃ → products.	RL	713	7.8(-2)			2/2	
71 BAL/LAN k _a + k _b .	RL	713	7.86(7)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
73 BAL/FUL k_a/k_{ref} . k_{ref} : $HO_2 + HCHO \rightarrow H_2O_2 + CHO$. Rate ratio per secondary C-H bond: $k_{sec}/k_{ref} = 0.024$	RL	773	4.8(-2)			2/2
73 BAL/FUL k_a . Rate constant per secondary C-H bond: $k_{sec} = 2.4 \times 10^7 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$	RN	773	4.8(7)			2
73 BAL/FUL k_b/k_{ref} . k_{ref} : $HO_2 + HCHO \rightarrow H_2O_2 + CHO$. Rate ratio per primary C-H bond: $k_{prim}/k_{ref} = 0.005$	RL	773	3.0(-2)			2/2
73 BAL/FUL k_b . Rate constant per primary C-H bond: $k_{prim} = 5.1 \times 10^6 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$	RN	773	3.06(7)			2
$HO_2 + CH_3CH_2CHO \rightarrow H_2O_2 + CH_3CH_2CO$ Hydroperoxo + Propanal						
71 BAL/LAN	ES	713	1.82(9)			2
79 BAL/LEW1 Oxidation in an aged boric-acid-coated-vessel.	RN	713	(1.52±0.15)(9)			2
$HO_2 + \text{trans-}CH_3CH=CHCH_3 \rightarrow \text{products}$ Hydroperoxo + 2-Butene, (E)-						
79 GRA/WIN Thermolysis of HO_2NO_2 . Upper-limit k. P(Total) = 760 torr.	EX	300	≤2.41(6)			2
$HO_2 + (CH_3)_3CH \rightarrow H_2O_2 + (CH_3)_3C$ (a) $\rightarrow H_2O_2 + (CH_3)_2CHCH_3$ (b) Hydroperoxo + Propane, 2-methyl-						
73 BAL/FUL k_a/k_{ref} . k_{ref} : $HO_2 + HCHO \rightarrow H_2O_2 + CHO$. Rate ratio per tertiary C-H bond: $k_{tert}/k_{ref} = 0.133$	RL	773	1.33(-1)			2/2
73 BAL/FUL k_a . Rate constant per tertiary C-H bond: $k_{tert} = 1.4 \times 10^8 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$	RN	773	1.35(8)			2
73 BAL/FUL k_b/k_{ref} . k_{ref} : $HO_2 + HCHO \rightarrow H_2O_2 + CHO$. Rate ratio per primary C-H bond: $k_{prim}/k_{ref} = 0.005$	RL	773	4.5(-2)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
73 BAL/FUL k _b . Rate constant per primary C-H bond: k _{prim} = 5.1x10 ⁶ cm ³ mol ⁻¹ s ⁻¹	RN	773	4.59(7)			2	
71 BAL/LAN (k _a + k _b)/k _{ref} . k _{ref} : HCHO + (CH ₃) ₃ CH → products.	RL	713	1.55(-1)			2/2	
73 BAL/FUL (k _a + k _b)/k _{ref} .	RL	773	1.78(-1)			2/2	
73 BAL/FUL k _a + k _b .	RN	773	1.81(8)			2	
HO ₂ + CH ₃ CH ₂ CH ₂ CHO → H ₂ O ₂ + CH ₃ CH ₂ CH ₂ CO Hydroperoxo + Butanal							
71 BAL/LAN	ES	713	2.41(9)			2	
HO ₂ + (CH ₃) ₂ CHCHO → H ₂ O ₂ + (CH ₃) ₂ CHCO (a) → H ₂ O ₂ + (CH ₃) ₂ CCHO (b) → H ₂ O ₂ + CH ₂ CH(CH ₃)CHO (c)							
Hydroperoxo + Propanal, 2-methyl-							
79 BAL/CLE ¹) k _a .	EX	713	(1.83±0.10)(9)			2	
79 BAL/CLE ¹) k _b .	EX	713	(1.4±0.2)(8)			2	
¹) Oxidation in an aged boric-acid-coated vessel. P(Total) = 60 Atm.							
HO ₂ + (CH ₃) ₂ C=C(CH ₃) ₂ → products Hydroperoxo + 2-Butene, 2,3-dimethyl-							
79 GRA/WIN Thermolysis of HO ₂ NO ₂ . Upper-limit k. P(Total) = 760 torr.	EX	300	≤2.41(7)			2	
HO ₂ + (CH ₃) ₂ CHCH(CH ₃) ₂ → H ₂ O ₂ + (CH ₃) ₂ CHC(CH ₃) ₂ Hydroperoxo + Butane, 2,3-dimethyl-							
75 ALC/MIL Optimization.	ES	373	2.5(5)			2	
77 ALC/MIL Azomethane photolysis. Optimization.	ES	373	2.5(5)			2	
H ₂ O (+ M) → H + OH (+ M) Water							
78 BOP/KER Shock-tube system. M = Ar/Kr mixture.	EX	3600-4800	1.26(14)	0	50327±1510	2	1.6

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$D_2O (+M) \rightarrow D + OD (+M)$							
Water-d ₂							
78 BOP/KER Shock-tube system. M = Ar/Kr mixture.	EX	3600-4800	1.26(14)	0	50327±1510	2	1.6
$H_2O + SO_3 \rightarrow H_2SO_4$							
Water + Sulfur trioxide							
75 CAS/DAV	EX	298	(5.48±1.20)(11)			2	
$H_2O + NO_2 \rightarrow OH + HONO$							
Water + Nitrogen oxide (NO ₂)							
76 FIF $k_1 = k_{-1}K$.	DE	1000-1380	8.3(12)	0	21138	2	
$H_2O + NO_2 + NO_2 \rightarrow HONO + HONO_2$							
Water + Nitrogen oxide (NO ₂)							
74 ENG/COR	EX	298	(5.50±0.29)(10)			3	
74 ENG/COR A and B recalculated from the reported data.	EX	298-323	(7.79±1.09)(9)	0	-580±43	3	1.1
79 STR/WEL Tunable diode-laser. Static reactor. Based on $k_1 = k_{-1}K$ and thermochemical data.	DE	296	2.90(9)			3	
$H_2O + N_2O_3 \rightarrow HNO_2 + HNO_2$							
Water + Nitrogen oxide (N ₂ O ₃)							
75 ENG/COR	RN	298	1.2(7)			2	
75 ENG/COR A and B recalculated from the reported data.	RN	313-323	(5.88±2.24)(13)	0	4605±120	2	
$H_2O + N_2O_4 \rightarrow HONO + HONO_2$							
Water + Nitrogen oxide (N ₂ O ₄)							
74 ENG/COR	EX	298	8.12(5)			2	
74 ENG/COR A and B recalculated from the reported data.	EX	298-323	(3.74±0.76)(14)	0	5954±64	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{H}_2\text{O} + \text{N}_2\text{O}_5 \rightarrow \text{HONO}_2 + \text{HONO}_2$ Water + Nitrogen oxide (N_2O_5)						
73 MOR/NIK2 Upper-limit k.	EX	298	$\leq 7.83(3)$			2
$\text{H}_2\text{O}_2 (+ \text{M}) \rightarrow \text{OH} + \text{OH} (+ \text{M})$ (a) → any other products (b) Hydrogen peroxide						
71 KIJ/TRO k_a . M = Ar. Shock waves.	EX	870-1400	1.58(16)	0	21641	2
79 BAS/KOG k_a . M = Ar. Flow-reactor.	EX	1095-1253	4.07(16)	0	21137±1761	2 4.5
71 TES/FOR	EX	717-754	3.16(18)	0	23553±654	2 2.51
$\text{H}_2\text{O}_2 + \text{NO} \rightarrow \text{OH} + \text{HONO}$ Hydrogen peroxide + Nitrogen oxide (NO)						
72 GRA/LIS Upper-limit k. The reaction is assumed to occur entirely in gas phase.	EX	298	$\leq 3.10(14)$			2
80 LIT IR-Absorption Spectroscopy. Upper-limit k. The reaction might be heterogeneous.	EX	263-283	$\leq 6.02(4)$			2
$\text{H}_2\text{O}_2 + \text{NO}_2 \rightarrow \text{HONO}_2 + 1/2\text{H}_2\text{O} + 1/4\text{O}_2$ (overall) Hydrogen peroxide + Nitrogen oxide (NO_2)						
72 GRA/LIS Upper-limit k.	ES	298	$\leq 6.0(5)$			2
$\text{H}_2\text{O}_2 + \text{N}_2\text{O}_5 \rightarrow \text{HOONO}_2 + \text{HONO}_2$ Hydrogen peroxide + Nitrogen oxide (N_2O_5)						
80 LIT IR-Absorption Spectroscopy. Upper limit k. P = (10-80) torr.	EX	253-283	$< 6.02(5)$			2
$\text{H}_2\text{O}_2 + \text{HONO}_2 \rightarrow \text{products}$ Hydrogen peroxide + Nitric acid						
80 LIT IR-Absorption Spectroscopy. Upper-limit k.	EX	263-283	$< 6.02(4)$			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
S + O₂ → SO + O							
Sulfur atom + Oxygen molecule							
71 FAI/VAN Flash photolysis. Vacuum-UV Kinetic Spectroscopy.	EX	298	(1.7±0.2)(12)			2	
72 DAV/KLE1	EX	252-423	(1.35±0.16)(12)	0	0±50	2	
72 DCN/LIT	EX	295	(1.0±0.2)(12)			2	
75 CLY/TOW	EX	298	(9.03±1.87)(11)			2	
79 CLY/WHI Resonance-fluorescence. Microwave-discharge.	EX	296-410	(1.02±0.30)(12)	0	-153±108	2	
S + O₃ → SO + O₂							
Sulfur atom + Ozone							
75 CLY/TOW	EX	298	(7.23±1.87)(12)			2	
S(¹D) + H₂ → products							
Sulfur atom + Hydrogen molecule							
72 LIT/DAL k _{ref} : S(¹ D) + CH ₂ =CH ₂ → products.	RL	300	2.2(-1)			2	
S + S (+ M) → S₂ (+ M)							
Sulfur atom							
79 NIC/AMO Radio-frequency pulse. Kinetic Spectroscopy. High-vacuum. Computer simulation. P = (0.1-2) torr.	DE	295	(4.3±0.6)(18)			3	
S + SH → S₂ + H							
Sulfur atom + Mercapto							
79 NIC/AMO Radio-frequency pulse. Kinetic Spectroscopy. High-vacuum. Computer simulation. P = (0.1-2) torr. Upper-limit k.	DE	295	<3.0(12)			2	
S(¹D) + N₂ → products							
Sulfur atom + Nitrogen molecule							
72 LIT/DAL k _{ref} : S(¹ D) + CH ₂ =CH ₂ → products.	RL	300	6.2(-2)			2/2	
S(¹D) + NO → products							
Sulfur atom + Nitrogen oxide (NO)							
72 LIT/DAL k _{ref} : S(¹ D) + CH ₂ =CH ₂ → products.	RL	300	6.8(-1)			2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
S + NO (+ M) → SNO (+ M)						
Sulfur atom + Nitrogen oxide (NO)						
78 VAN/OBI ¹⁾ M = CO ₂ . Low-pressure k. P(CO ₂) <100 torr.	EX	298	(1.9±0.1)(17)			3
78 VAN/OBI ¹⁾ M = CO ₂ . Limiting high-pressure k.	EX	298	(9.3±2.1)(12)			2
¹⁾ Flash-photolysis. Vacuum-UV Absorption Spectroscopy.						
S + NO₂ → SO + NO						
Sulfur atom + Nitrogen oxide (NO ₂)						
75 CLY/TOW	EX	298	(3.73±0.85)(13)			2
79 CLY/WHI Resonance-fluorescence. Microwave-discharge.	EX	296-410	(2.95±0.60)(13)	0	-84±60	2
S(¹D) + N₂O → NS + NO						
Sulfur atom + Nitrogen oxide (N ₂ O)						
72 LIT/DAL k _{ref} : S(¹ D) + CH ₂ =CH ₂ → products.	RL	300	≈1.0(-1)			2/2
S(¹D) + CO → products						
Sulfur atom + Carbon monoxide						
72 LIT/DAL k _{ref} : S(¹ D) + CH ₂ =CH ₂ → products.	RL	300	1.9(-1)			2/2
S(¹D) + CO₂ → products						
Sulfur atom + Carbon dioxide						
72 LIT/DAL k _{ref} : S(¹ D) + CH ₂ =CH ₂ → products.	RL	300	2.4(-1)			2/2
S(¹D) + CH₄ → CH₃SH						
Sulfur atom + Methane						
72 LIT/DAL k _{ref} : S(¹ D) + CH ₂ =CH ₂ → products.	RL	300	7.6(-2)			2/2
80 ADD/DON CS ₂ photolysis. Time-Resolved Resonance-fluorescence.	EX	295	(1.08±0.18)(14)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
S + COS → S₂ + CO							
Sulfur atom + Carbon oxide sulfide							
72 JAK/AHM	RL	298	8.3(1)				2/2
$k_{ref}: S + CH_2=CH_2 \rightarrow \triangle S$							
72 JAK/AHM	RN	298	1.1(10)				2
74 KLE/DAV	EX	233-445	(9.15±1.20)(11)	0	1827±60		2
S(¹D) + COS → S₂ + CO							
Sulfur atom + Carbon oxide sulfide							
72 LIT/DAL	RL	300	(1.5±0.5)				2/2
$k_{ref}: S(^1D) + CH_2=CH_2 \rightarrow \text{products.}$							
79 ADD/BYR	EX	290	(7.23±1.81)(13)				2
COS UV-photolysis. Time-Resolved Atomic Absorption Spectroscopy.							
79 SHE/SAF ¹⁾	RL	298	2.4				2/2
$k_{ref}: S(^1D) + COS \rightarrow S + COS.$							
79 SHE/SAF ¹⁾	RL	298	5.7(-1)				2/2
$k_{ref}: S(^1D) + CH_2=CH_2 \rightarrow CH_2=CHSH \quad (a)$							
$\rightarrow \triangle S^\dagger \quad (b)$							
$(k_{ref} = k_a + k_b.)$							
¹⁾ UV-photolysis of COS in a high-vacuum system. Optimization.							
80 ADD/DON	EX	295	(1.81±0.60)(14)				2
CS ₂ photolysis. Time-Resolved Resonance-Fluorescence.							
S + CH=CH → $\triangle S$ (a)							
→ :CHCHS[†] (b)							
Sulfur atom + Ethyne							
71 STR/O'C	RL	298-450	6.2	0	1007		2/2
$k_a/k_{ref}.$ Conventional photolysis method.							
$k_{ref}: S + CH_2=CH_2 \rightarrow \triangle S$							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
73 LIT/DON k _a . Flash-photolysis of COS in Ar. P(COS) = 0.1 torr. P(Ar) = 150 torr.	EX	295	(3.01±0.30)(11)			2
78 VAN/SAF ¹⁾	EX	298	(2.3±0.4)(11)			2
78 VAN/SAF ¹⁾ ¹⁾ k _b . Flash-photolysis. Vacuum-UV Absorption Spectroscopy. A spin-allowed, least motion primary path is assumed.	EX	298-484	(3.4±1.9)(13)	0	1510±201	2
S(¹ D) + CH≡CH → Δ						
Sulfur atom + Ethyne						
73 LIT/DON COS Flash-photolysis in Ar. k _{ref} : S(¹ D) + CO ₂ → S(³ P) + CO ₂ . P(Ar) = 150 torr.	RL	295	(2.5±0.4)			2/2
S + CD≡CD → :CDCDS [†]						
Sulfur atom + Ethyne-d ₂						
78 VAN/SAF Flash-photolysis. Vacuum-UV Absorption Spectroscopy. A spin-allowed, least motion primary path is assumed.	EX	298	(2.3±0.4)(11)			2
S + CH ₂ =CH ₂ → Δ						
Sulfur atom + Ethene						
71 CON/VAN Flash-photolysis method.	EX	298	(9.0±1.0)(11)			2
71 STR/O'C Conventional photolysis method.	ES	298-450	≤1.0(13)	0	755	2
72 DAV/KLE2	ES	218-442	(4.29±0.45)(12)	0	795±40	2
S + CH ₂ =CD ₂ → Δ _{D₂}						
Sulfur atom + Ethene-1,1-d ₂						
71 STR/O'C Conventional photolysis method.	RL	298-450	1.07	0	0	2/2
k _{ref} : S + CH ₂ =CH ₂ → Δ						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$S + \text{cis-CHD=CHD} \rightarrow \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \\ \text{D} \quad \text{D} \end{array}$						
Sulfur atom + Ethene-1,2-d ₂ , (Z)-						
71 STR/O'C Conventional photolysis method.	RL	298-450	1.04	0	0	2/2
$k_{\text{ref}}: S + \text{CH}_2=\text{CH}_2 \rightarrow \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \end{array}$						
$S + \text{CD}_2=\text{CD}_2 \rightarrow \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \\ \text{D} \quad \text{D} \end{array}$						
Sulfur atom + Ethene-d ₄						
71 STR/O'C Conventional photolysis method.	RL	298-450	1.14	0	0	2/2
$k_{\text{ref}}: S + \text{CH}_2=\text{CH}_2 \rightarrow \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \end{array}$						
$S(^1\text{D}) + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHSH} \quad (\text{a})$						
$\rightarrow \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \end{array} \quad (\text{b})$						
Sulfur atom + Ethene						
79 SHE/SAF ¹⁾ k_a .	RN	298	4.2(13)			2
79 SHE/SAF ¹⁾ k_b .	DE	298	3.8(13)			2
¹⁾ UV-photolysis of COS. Optimization.						
$S(^1\text{D}) + \text{CH}_3\text{CH}_3 \rightarrow \text{products}$						
Sulfur atom + Ethane						
72 LIT/DAL $k_{\text{ref}}: S(^1\text{D}) + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHSH} \quad (\text{a})$ $\rightarrow \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \end{array} \quad (\text{b})$	RL	300	1.7(-1)			2/2
$S + \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \end{array} \rightarrow \text{S}_2 + \text{CH}_2=\text{CH}_2$						
Sulfur atom + Thiirane (Ethylene episulfide)						
71 STR/O'C Conventional photolysis method.	RL	298-450	8.3	0	-906	2/2
$k_{\text{ref}}: S + \text{CH}_2=\text{CH}_2 \rightarrow \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \end{array}$						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$S + CH_3C\equiv CH \rightarrow$ $H_3C-\triangle^S$ (a)						
$\rightarrow :C(CH_3)CHS^\dagger$ (b)						
Sulfur atom + 1-Propyne						
71 STR/O'C	RL	298-450	6.2	0	453	2/2
k_a/k_{ref} . Conventional photolysis.						
$k_{ref}: S + CH_2=CH_2 \rightarrow \triangle^S$						
78 VAN/SAF ¹⁾	EX	298	(4.8±0.2)(12)			2
78 VAN/SAF ¹⁾	EX	298-449	(2.0±1.2)(13)	0	453±101	2
¹⁾ k_p . Flash-photolysis.						
Absorption spectroscopy. A spin-allowed, least motion primary path assumed.						
$S + CH_3CH=CH_2 \rightarrow$ $H_3C-\triangle^S$						
Sulfur atom + 1-Propene						
71 CON/VAN ¹⁾	RL	298	(7.5±1.3)			2/2
$k_{ref}: S + CH_2=CH_2 \rightarrow \triangle^S$						
71 CON/VAN ¹⁾	RN	298	(6.0±1.0)(11)			2
¹⁾ Flash-photolysis.						
71 STR/O'C	RL	298-450	1.0	0	-574	2/2
Conventional photolysis.						
$k_{ref}: S + CH_2=CH_2 \rightarrow \triangle^S$						
73 KLE/DAV2	EX	214-500	(3.63±0.43)(12)	0	191±45	2
$S +$ $H_3C-\triangle^S$ $\rightarrow S_2 + CH_3CH=CH_2$						
Sulfur atom + Thiirane, methyl-						
71 STR/O'C	RL	298-450	8.4	0	-1057	2/2
Conventional photolysis.						
$k_{ref}: S + CH_2=CH_2 \rightarrow \triangle^S$						
$S + CH_3CH_2C\equiv CH \rightarrow :C(CH_2CH_3)CHS^\dagger$						
Sulfur atom + 1-Butyne						
78 VAN/SAF	EX	298	(3.3±0.2)(12)			2
Flash-photolysis.						
Absorption Spectroscopy. A spin allowed, least motion primary path assumed.						

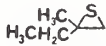
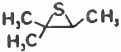
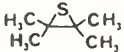
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$S + CH_3C\equiv CCH_3 \rightarrow H_3C-\triangle-S-CH_3$ (a) $\rightarrow :C(CH_3)C(S)CH_3^\dagger$ (b) Sulfur atom + 2-Butyne 71 STR/O'C k_a/k_{ref} Conventional photolysis. k_{ref} : $S + CH_2=CH_2 \rightarrow \triangle S$	RL	298-450	2.7	0	-654	2/2	
78 VAN/SAF k_b . Flash-photolysis. Absorption-spectroscopy. A spin-allowed, least motion primary path assumed.	EX	298	(1.6±0.2)(13)			2	
$S + CH_2=CHCH=CH_2 \rightarrow H_2C=HC-\triangle S$ Sulfur atom + 1,3-Butadiene 71 STR/O'C Conventional photolysis. k_{ref} : $S + CH_2=CH_2 \rightarrow \triangle S$	RL	298-450	2.4	0	-1027	2/2	
$S + CH_3CH_2CH=CH_2 \rightarrow H_3CH_2C-\triangle S$ Sulfur atom + 1-Butene 71 CON/VAN ¹⁾ k_{ref} : $S + CH_2=CH_2 \rightarrow \triangle S$	RL	298	(1.1±0.2)(1)			2/2	
71 CON/VAN ¹⁾ ¹⁾ Flash-photolysis method.	RN	298	(9.1±1.0)(12)			2	
71 STR/O'C Conventional photolysis. k_{ref} : $S + CH_2=CH_2 \rightarrow \triangle S$	RL	298-450	7.5(-1)	0	-866	2/2	
73 KLE/DAV2	EX	216-475	(4.46±0.69)(12)	0	181±45	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$S + \text{cis-CH}_3\text{CH=CHCH}_3 \rightarrow$  Sulfur atom + 2-Butene, (Z)- 71 STR/O'C Conventional photolysis. $k_{\text{ref}}:$	RL	298-450	5.3(-1)	0	-1052	2/2
$S + \text{CH}_2=\text{CH}_2 \rightarrow$  73 DAV/KLE $S + \text{trans-CH}_3\text{CH=CHCH}_3 \rightarrow$  Sulfur atom + 2-Butene, (E)- 71 CON/VAN ¹⁾ $k_{\text{ref}}:$	EX	219-500	(2.82±0.42)(12)	0	-116±45	2
$S + \text{CH}_2=\text{CH}_2 \rightarrow$  71 CON/VAN ¹⁾ ¹⁾ Flash-photolysis method. 71 STR/O'C Conventional photolysis. $k_{\text{ref}}:$	RL	298	(1.5±0.3)(1)			2/2
$S + \text{CH}_2=\text{CH}_2 \rightarrow$  $S + (\text{CH}_3)_2\text{C=CH}_2 \rightarrow$  Sulfur atom + 1-Propene, 2-methyl- 71 CON/VAN ¹⁾ $k_{\text{ref}}:$	RN	298	(1.2±0.2)(13)			2
$S + \text{CH}_2=\text{CH}_2 \rightarrow$  71 CON/VAN ¹⁾ ¹⁾ Flash-photolysis. 71 STR/O'C Conventional photolysis. $k_{\text{ref}}:$	RL	298-450	6.5(-1)	0	-1012	2/2
$S + \text{CH}_2=\text{CH}_2 \rightarrow$  71 CON/VAN ¹⁾ ¹⁾ Flash-photolysis. 71 STR/O'C Conventional photolysis. $k_{\text{ref}}:$	RL	298	(4.5±0.6)(1)			2/2
$S + \text{CH}_2=\text{CH}_2 \rightarrow$  71 CON/VAN ¹⁾ ¹⁾ Flash-photolysis. 71 STR/O'C Conventional photolysis. $k_{\text{ref}}:$	RL	298-450	(3.6±0.5)(13)			2
$S + \text{CH}_2=\text{CH}_2 \rightarrow$  71 CON/VAN ¹⁾ ¹⁾ Flash-photolysis. 71 STR/O'C Conventional photolysis. $k_{\text{ref}}:$	RL	298-450	9.7(-1)	0	-1188	2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$S + CH_3CH_2C \equiv CH_3 \rightarrow :C(CH_3)C(S)CH_2CH_3^\ddagger$ (a) $\rightarrow :C(CH_2CH_3)C(S)CH_3^\ddagger$ (b)						
Sulfur atom + 2-Pentyne						
78 VAN/SAF	EX	298	(1.8±0.2)(13)			2
$k_a + k_b$. Flash-photolysis. Absorption Spectroscopy. A spin-allowed, least motion primary path assumed.						
$S + $  $\rightarrow $ 						
Sulfur atom + Cyclopentene						
71 STR/O'C	RL	298-450	6.7(-1)	0	-1082	2/2
Conventional photolysis.						
$k_{ref}: S + CH_2=CH_2 \rightarrow $ 						
$S + CH_3CH_2C(CH_3)=CH_2 \rightarrow $ 						
Sulfur atom + 1-Butene, 2-methyl-						
71 STR/O'C	RL	298-450	7.8(-1)	0	-1424	2/2
Conventional photolysis.						
$k_{ref}: S + CH_2=CH_2 \rightarrow $ 						
$S + (CH_3)_2C=CHCH_3 \rightarrow $ 						
Sulfur atom + 2-Butene, 2-methyl-						
71 STR/O'C	RL	298-450	5.1(-1)	0	-1515	2/2
Conventional photolysis.						
$k_{ref}: S + CH_2=CH_2 \rightarrow $ 						
$S + (CH_3)_2C=C(CH_3)_2 \rightarrow $ 						
Sulfur atom + 2-Butene, 2,3-dimethyl-						
71 CON/VAN ¹)	RL	298	(7.7±1.0)(1)			2/2
$k_{ref}: S + CH_2=CH_2 \rightarrow $ 						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
71 CON/VAN ¹⁾ Lower-limit k. ¹⁾ Flash-photolysis.	RN	298	$\geq(6.2 \pm 0.8)(13)$			2	
71 STR/O'C Conventional photolysis. $k_{\text{ref}}: \text{S} + \text{CH}_2=\text{CH}_2 \rightarrow \text{S}_2$	RL	298-450	5.0(-1)	0	-1691	2/2	
73 DAV/KLE	EX	252-500	$(2.82 \pm 1.02)(12)$	0	-649 $\pm$ 116	2	
S₂ (+ M) → S + S (+ M)							
Sulfur dimer							
80 HIG/SAI M = Ar. COS pyrolysis behind incident shock-waves. Possibly an upper-limit k. P = (240-380) torr.	EX	4500-6000	4.79(13)	0	38752	2	
S₂ + S₂ (+ M) → S₄ (+ M)							
Sulfur dimer							
72 LAN/OLD M = CO ₂ .	ES	293	9.07(17)			3	10.0
73 LAN/OLD M = CO ₂ .	ES	293	3.6(18)			3	5.0
79 NIC/AMO Radio-frequency pulse. Kinetic Spectroscopy. High-vacuum. k determined by computer simulation. P = (0.1-2) torr.	DE	295	$(8.0 \pm 1.0)(18)$			3	
SO (+ M) → S + O (+ M)							
Sulfur monoxide							
78 AST/GLA M = Ar. Incident or reflected shock-waves. Rate constant expressed as k[Ar].	EX	5700-7200	1.58(14)	0	55331 $\pm$ 3608	2	4.0
SO + O₂ → SO₂ + O							
Sulfur monoxide + Oxygen molecule							
72 BRE/MIL Fast-flow. EPR detection. Upper-limit k. P(Total) = 0.45 torr.	EX	297	<5.0(7)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 BLA/SHA1 ¹⁾	EX	298	(6.44±0.96)(7)			2
82 BLA/SHA2 ¹⁾	EX	230-420	1.44(11)	0	2370±250	2 2.1
¹⁾ ArF Laser-photodissociation of SO ₂ at 193 nm. in He. P(He) < 400 torr. P(SO ₂) ~ 30 mtorr. P(O ₂) < 500 torr.						
SO + SO (+ M) → SO ₂ + S (+ M)						
Sulfur monoxide						
72 BRE/MIL	EX	297	<3.0(10)			2
Fast-flow technique with EPR detection. P(Total) = 0.45 torr. Upper-limit k.						
75 CHU/CAL	ES	298	(5.0±4.0)(8)			2
Best fit.						
80 HER/HUI	EX	298	1.6(17)			3
M = N ₂ . Tubular flow-reactor. Mass-spectrometry.						
SO + SO ₃ → SO ₂ + SO ₂						
Sulfur monoxide + Sulfur trioxide						
75 CHU/CAL	ES	298	(1.2±0.7)(9)			2
Best fit.						
SO + (SO) ₂ → SO ₂ + S ₂ O						
Sulfur monoxide + Sulfur monoxide dimer						
80 HER/HUI	EX	298	2.0(10)			2
Tubular flow-reactor. Mass-spectrometry.						
SO + NO ₂ → SO ₂ + NO						
Sulfur monoxide + Nitrogen oxide (NO ₂)						
71 MIY/TAK2	EX	298	(1.23±0.15)(12)			2
80 CLY/MAC	EX	295	(8.19±0.60)(12)			2
Discharge-flow. Mass-spectrometry.						
82 BLA/SHA1	EX	298	(8.91±1.20)(12)			2
ArF Laser-photodissociation of SO ₂ at 193 nm. in presence of diluent gas. P(He) = (100-500) torr. P(SO ₂) ~ 30 mtorr.						
SO ₂ (+ M) → SO + O (+ M)						
Sulfur dioxide						
75 KIE	EX	2900-5200	1.70(16)	0	56366±2013	2
M = Kr. Incident shock-waves. (3-30)% SO ₂ and (70-97)% Kr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 AST/GLA M = Ar. Incident or reflected shock-waves. [Ar] = (0.3-4.0)x10 ¹⁹ molec.cm ⁻³ Rate constant expressed as k[Ar].	EX	3700-7500	3.98(14)	0	53888±2165	2	2.0
78 JUS/RIM M = Ar. Reflected shock-waves.	EX	2500-3400	2.9(16)	0	58590±2270	2	2.2
79 GRI/REE ¹⁾ Total dens.: (0.5-2.0)x10 ¹⁹ molec.cm ⁻³ .	EX	2800-3880	(8.0±2.0)(15)	0	54353	2	
79 GRI/REE ¹⁾ Extended T-range, for M = Ar, or Kr. About a factor of 20 above literature values.	SE	2500-5200	1.5(16)	0	56366	2	
¹⁾ M = Ar. Reflected shock-waves.							
80 RAJ/BAB ²⁾ M = Ar.	EX	4000-6000	3.34(15)	0	54152	2	
80 RAJ/BAB ²⁾ M = SO ₂ .	EX	4000-6000	5.02(14)	0	33518	2	
²⁾ Thermolysis of SO ₂ behind incident shock-waves. P = (1.0-2.5) torr.							
80 SAI/YOK2 M = Ar. Thermolysis of SO ₂ behind reflected shock-waves. Total dens. = (0.5-1.4)x10 ¹⁸ molec.cm ⁻³ .	EX	4300-6200	3.55(14)	0	52805	2	
82 RAJ/BAB ³⁾ M = Ar.	EX	4000-6000	3.34(15)	0	54152	2	
82 RAJ/BAB ³⁾ M = SO ₂ .	EX	4000-6000	5.02(14)	0	33518	2	
³⁾ Dissociation of SO ₂ behind incident shock-waves, in Ar. Gas-chromatography. P ₀ = (1.0-2.5) torr.							
 SO ₂ + SO ₂ (¹ B ₁) → SO(¹ Δ _g , ³ Σ ⁻) + SO ₃ Sulfur dioxide							
75 CHU/CAL	ES	298	(2.2±0.5)(12)			2	
 SO ₂ + SO ₂ (³ B ₁) → SO(³ Σ ⁻) + SO ₃ Sulfur dioxide							
75 CHU/CAL	ES	298	(4.2±0.4)(10)			2	
 SO ₂ + NO ₂ → SO ₃ + NO Sulfur dioxide + Nitrogen oxide (NO ₂)							
71 ARM/CUL	EX	703-1193	6.31(12)	0	13588	2	
77 FRE/PAL	EX	703-1850	6.31(12)	0	13588	2	
Extended validity of k reported in 71 ARM/CUL.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{SO}_2 + \text{NO}_3 \rightarrow \text{SO}_3 + \text{NO}_2$						
Sulfur dioxide + Nitrogen dioxide (NO_2)						
75 DAU/CAL Upper-limit k.	ES	300	$\leq 4.2(3)$			2
$\text{SO}_2 + \text{N}_2\text{O}_5 \rightarrow \text{SO}_3 + \text{N}_2\text{O}_4$						
Sulfur dioxide + Nitrogen oxide (N_2O_5)						
75 DAU/CAL Upper-limit k.	ES	300	$\leq 2.5(1)$			2
$\text{SO}_2 + \text{CO} \rightarrow \text{products}$						
Sulfur dioxide + Carbon monoxide						
71 BAU/JEF M = Ar. P = (27-170) torr.	EX	1770-2453	2.69(12)	0	24303±604	2 1.32
$\text{SO}_2^* + \text{CO} \rightarrow \text{SO} + \text{CO}_2$						
Sulfur dioxide + Carbon monoxide						
73 CEH/HEI ¹⁾ At 2537 A ₀ .	RL	300	5.0(-4)			2/2
73 CEH/HEI ¹⁾ At 3130 A ₀ .	RL	300	1.5(-3)			2/2
73 CEH/HEI ¹⁾ At 3130-3261 A ₀ . The rate ratio to be multiplied by a factor α , dependent on the experimental conditions.	RL	300	4.12(2)			2/1
¹⁾ k _{ref} : $\text{SO}_2^* \rightarrow \text{products}$. SO ₂ * is a vibrationally excited singlet.						
$\text{SO}_2^{**} + \text{CO} \rightarrow \text{SO} + \text{CO}_2$						
Sulfur dioxide + Carbon monoxide						
73 CEH/HEI ¹⁾ At 2536 A ₀ .	RL	300	2.24(2)			2/1 1.4
73 CEH/HEI ¹⁾ At 3130 A ₀ .	RL	300	3.37(2)			2/1 1.4
73 CEH/HEI ¹⁾ At 3261 A ₀ .	RL	300	4.68(2)			2/1 1.4
¹⁾ k _{ref} : $\text{SO}_2^{**} \rightarrow \text{SO}_2$. SO ₂ ^{**} is a chemically active triplet. The rate ratio to be multiplied by a factor β , depending on the experimental conditions.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{SO}_2 + \text{CH}=\text{CH} \rightarrow \text{CO} + \text{other products}$						
Sulfur dioxide + Ethyne						
71 FIF/MOR	ES	1500-2150	5.46(11)	0.5	20533	2
The preexponential factor expressed as: $A(T/298)^{0.5}$.						
$\text{SO}_2(^3\text{B}_1) + \text{CH}=\text{CH} \rightarrow \text{CO} + \text{other products}$						
Sulfur dioxide + Ethyne						
77 SU/CAL	EX	298	1.56(12)			2
Photolysis of $\text{SO}_2/\text{CH}=\text{CH}$ mixtures.						
$\text{SO}_2(^3\text{B}_1) + \text{cis-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow [\text{cis-CH}_3\text{CH}=\text{CHCH}_3.\text{SO}_2]^*$						
Sulfur dioxide + 2-Butene, (Z)-						
74 DEM/CAL	ES	294	(1.29±0.18)(14)			2
$\text{SO}_2(^3\text{B}_1) + \text{trans-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow [\text{trans-CH}_3\text{CH}=\text{CHCH}_3.\text{SO}_2]^*$						
Sulfur dioxide + 2-Butene, (E)-						
74 DEM/CAL	ES	294	(1.22±0.15)(14)			2
$\text{SO}_2(^1\text{B}_1) + (\text{CH}_3)_3\text{CH} \rightarrow \text{products}$						
Sulfur dioxide + Propane, 2-methyl-						
78 SU/CAL	EX	298	8.4(12)			2
SO_2 photolysis. P < 10 torr.						
$\text{SO}_2(^3\text{B}_1) + (\text{CH}_3)_3\text{CH} \rightarrow \text{products}$						
Sulfur dioxide + Propane, 2-methyl-						
78 SU/CAL	EX	298	8.7(11)			2
SO_2 photolysis. P < 10 torr.						
$\text{SO}_2(^3\text{B}_1) + \text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow [\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3.\text{SO}_2]^*$						
$\rightarrow \text{SO}_2 + \text{trans-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3$						
Sulfur dioxide + 2-Pentene, (Z)-						
76 WAM	ES	295	(6.33±1.25)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{SO}_2(^3\text{B}_1) + \text{trans-CH}_3\text{CH}_2\text{CH=CHCH}_3$ $\rightarrow [\text{CH}_3\text{CH}_2\text{CH=CHCH}_3\cdot\text{SO}_2]^*$ $\rightarrow \text{SO}_2 + \text{cis-CH}_3\text{CH}_2\text{CH=CHCH}_3$						
Sulfur dioxide + 2-Pentene, (E)-						
76 WAM	ES	295	(1.0±0.27)(14)			2
$\text{SO}_3 (+\text{M}) \rightarrow \text{SO}_2 + \text{O} (+\text{M})$						
Sulfur trioxide						
79 AST/GLA	EX	1700-2500	3.16(15)	0	31875±1323	2 1.6
M = Ar. Incident or reflected shock-waves.						
k expressed as k[Ar]. Supersedes 78 AST/GLA.						
[Ar] = (0.5-4.2)×10 ¹⁹ molec.cm ⁻³ .						
$\text{SH} + \text{D}_2 \rightarrow \text{HDS} + \text{D}$						
Mercapto + Deuterium molecule						
77 PRA/ROG	EX	808-937	1.35(13)	0	3530±220	2 1.8
Static system.						
$\text{SH} + \text{SH} \rightarrow \text{H}_2\text{S} + \text{S}$						
Mercapto						
72 LAN/OLD	ES	293	≤1.81(13)			2
Upper-limit k.						
73 BRA/TRU	EX	298	7.8(12)			2
79 NIC/AMO	DE	295	(1.9±0.2)(13)			2
Radio-frequency pulse. Kinetic Spectroscopy.						
High-vacuum.						
P = (0.1-2) torr.						
$\text{SH} + \text{NO} \rightarrow \text{products}$						
Mercapto + Nitrogen oxide (NO)						
73 BRA/TRU	RN	298	6.3(11)			2
$\text{H}_2\text{S} (+\text{M}) \rightarrow \text{SH} + \text{H} (+\text{M})$						
Hydrogen sulfide						
76 HIG/SAI ¹⁾	ES	2380-3010	1.26(16)	0	46301	2
77 BOW/DOD ¹⁾	EX	2700-3800	2.00(14)	0	37288±962	2 1.51
82 ROT/LOE1 ¹⁾	EX	1965-2560	4.64(14)	0	41500	2
Thermolysis behind reflected shock-waves.						
Atomic Resonance Absorption-Spectroscopy.						
[H ₂ S] = (0.6-4.9)×10 ¹⁵ molec.cm ⁻³ .						
[Ar] = (5.0-8.0)×10 ¹⁸ molec.cm ⁻³ .						
P(Total) = (1350-1500) torr.						
¹⁾ M = Ar.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$N(^4S) + O_2 \rightarrow NO(v=n) + O$							
Nitrogen atom + Oxygen molecule							
81 RAH/GIB ¹⁾ n = 2.	EX	298	(3.31±0.84)(6)			2	
81 RAH/GIB ¹⁾ n = 3.	EX	298	(3.43±0.54)(6)			2	
81 RAH/GIB ¹⁾ n = 4.	EX	298	(1.99±0.18)(6)			2	
81 RAH/GIB ¹⁾ n = 5.	EX	298	(1.45±0.24)(6)			2	
81 RAH/GIB ¹⁾ n = 6.	EX	298	(4.22±1.20)(5)			2	
81 RAH/GIB ¹⁾ n = 7.	EX	298	(3.01±1.20)(5)			2	
¹⁾ Fourier Transform IR Spectrometry. P(N ₂) = 250 mtorr. P(O ₂) = 500 mtorr.							
$N(^2D) + O_2 \rightarrow NO + O$							
Nitrogen atom + Oxygen molecule							
71 LIN/KAU	EX	300	(3.61±1.20)(12)			2	
71 SLA/WOO	EX	237	4.94(12)			2	
71 SLA/WOO	EX	295	4.46(12)			2	
71 SLA/WOO	EX	365	5.18(12)			2	
71 SLA/WOO	EX	1000	8.43(12)			2	
Extrapolated rate constant.							
71 SLA/WOO The A-factor recalculated from the given T ^{0.5} term and the above experimental rate constants. The preexponential factor expressed as: A(T/298) ^{0.5} .	EX	237-365	4.68(12)	0.5	0	2	
72 HUS/KIR2	EX	300	(5.60±1.33)(12)			2	
$N(^2P) + O_2 \rightarrow NO + O$							
Nitrogen atom + Oxygen molecule							
72 HUS/KIR2	EX	300	(2.77±1.51)(12)			2	
$N + O_2(^1A_g) \rightarrow NO + O$							
Nitrogen atom + Oxygen molecule							
73 SCH/SCH2	EX	300	(1.35±0.52)(9)			2	
73 SCH/SCH2	SE	300	1.63(9)			2	
Average of present and literature data.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
N + O₃ → NO + O₂						
Nitrogen atom + Ozone						
79 STI/PAY Discharge-flow. Flash-photolysis. Resonance-fluorescence. Upper-limit k.	EX	298	<3.01(8)			2
N(²D) + O₃ → NO + O₂						
Nitrogen atom + Ozone						
80 HUS/SLA2 UV-photolysis of N ₂ O. Time-resolved Resonance-Fluorescence. Lower-limit k.	EX	300	>2.41(12)			2
N(²D) + H₂ → NH + H						
Nitrogen atom + Hydrogen molecule						
72 HUS/KIR2	EX	300	(1.02±0.30)(12)			2
N + H₂ (+ M) → NH₂ (+ M)						
Nitrogen atom + Hydrogen molecule						
81 PET/SAP Discharge-flow. N atoms produced by dissociation of N ₂ in a glow-discharge. Unreported T assumed to be 298 K. Upper-limit k. [H ₂] ~1.3x10 ¹⁷ molec.cm ⁻³ . [M] = 3.6x10 ¹⁷ molec.cm ⁻³ . P(H ₂) = (0.2-0.4) torr.	EX	298	≤3.63(11)			3
N + OH → NO + H						
Nitrogen atom + Hydroxyl						
77 HAY1 Fuel-rich, Ethylene-, and Acetylene-air flames. k _{ref} : N + NO → N ₂ + O.	RL	1950-2380	(1.0±0.2)			2/2
80 HOW/SMI Discharge-flow. H ₂ O Flash-photolysis. Resonance-fluorescence. P(Total) = 3.75 torr.	EX	298	(3.01±0.72)(13)			2
81 HOW/SMI Discharge-flow. OH radicals formed by H ₂ O Flash- photolysis. N atoms formed by dissociation of ~1% N ₂ in Ar. Resonance-fluorescence. The pre- exponential factor expressed as: A(T/298) ^{-0.25} . [N] = (0.5-5.1)x10 ¹³ molec.cm ⁻³ .	EX	250-515	(3.20±0.27)(13)	-0.25	0	2
81 MOR2 Premixed H ₂ /O ₂ /Ar flames. Laser-fluorescence. P = 760 torr. k _{ref} : N + NO → N ₂ + O.	RL	1790-2200	(1.0±0.3)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$N(^2D) + H_2O \rightarrow \text{products}$						
Nitrogen atom + Water						
76 SLA/BLA3 Vacuum UV-Photolysis. P(He) = 7 torr. P(N ₂ O + Ar) = 7 torr. (1% N ₂ O in Ar).	EX	198-372	(1.51±0.30)(14)			2
$N + SO_3 \rightarrow NO + SO_2$						
Nitrogen atom + Sulfur trioxide						
72 JAC/WIN	EX	300	3.07(8)			2
75 WES/DEH1 Upper-limit k.	EX	298	≤6.0(6)			2
$N + N (+ M) \rightarrow N_2 (+ M)$						
Nitrogen atom						
75 BED/TCH M = N ₂ . Electron Paramagnetic Resonance. P = (2.2-3.2) torr.	EX	298	(7.58±1.96)(15)			3
78 EME/MAR ¹⁾ M = Ar.	EX	300	(8.34±1.81)(15)			3
78 EME/MAR ¹⁾ M = He.	EX	300	(7.98±0.73)(15)			3
78 EME/MAR ¹⁾ M = N ₂ .	EX	300	(3.99±1.45)(15)			2
¹⁾ ESR-jet-flow technique. P(Total) = (1.5-8.0) torr.						
79 YAM M = N ₂ . Recombination of N atoms in Lewis-Rayleigh Nitrogen afterglow. P(N ₂) < 4.2 torr.	EX	298	(2.61±0.07)(15)			3
$N + NO \rightarrow N_2 + O$						
Nitrogen atom + Nitrogen oxide (NO)						
75 CLY/MCD	EX	298-670	(4.94±0.84)(13)	0	410±120	2
75 CLY/MCD	EX	298	(1.33±0.84)(13)			2
78 LEE/MIC3 Discharge-flow, or Flash-photolysis. Resonance-Fluorescence. T-independent k.	EX	196-400	(2.41±0.12)(13)	0	0	2
79 ISH/SUG1 Pulse-radiolysis. Absorption-spectroscopy. P(Total) = (200-800) torr.	EX	298	(1.39±0.24)(13)			2
80 CHE/CLY Discharge-flow. Resonance-fluorescence.	EX	298	(2.04±0.18)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 SUG/ISH2 Pulse-radiolysis. Resonance-absorption. P(Total) = (200-1000) torr.	EX	298	(1.14±0.12)(13)			2
N(²D) + NO → N₂ + O						
Nitrogen atom + Nitrogen oxide (NO)						
71 LIN/KAU	EX	300	(4.22±1.51)(13)			2
72 HUS/KIR2	EX	300	(3.67±2.23)(13)			2
80 SUG/ISH2 Pulse-radiolysis. Resonance-absorption. P(Total) = (200-1000) torr.	EX	298	(2.11±0.18)(13)			2
N(²P) + NO → N₂ + O						
Nitrogen atom + Nitrogen oxide (NO)						
72 HUS/KIR2	EX	300	(2.05±0.66)(13)			2
80 SUG/ISH2 Pulse-radiolysis. Resonance-absorption. P(Total) = (200-1000) torr.	EX	298	(1.63±0.12)(13)			2
N + NO₂ → N₂O + O (a)						
→ NO + NO (b)						
→ N ₂ + O ₂ (c)						
→ N ₂ + O + O (d)						
Nitrogen atom + Nitrogen oxide (NO ₂)						
75 CLY/MCD k _a .	EX	298	(8.43±0.12)(11)			2
82 CLY/ONO k _a + k _b + k _c + k _d . NO ₂ in excess. Discharge-flow. Resonance-fluorescence. [NO ₂]/[N] ₀ > 80.	EX	293	(1.81±0.19)(12)			2
N(²D) + N₂O → N₂ + NO (a)						
→ N(⁴ S) + N ₂ + O (b)						
Nitrogen atom + Nitrogen oxide (N ₂ O)						
71 SLA/WOO ¹⁾ Preexponential factor expressed as: A(T/298) ^{0.5} .	EX	237-365	3.75(12)	0.5	403±101	2
71 SLA/WOO ¹⁾	EX	300	1.02(12)			2
72 HUS/KIR2 ¹⁾	EX	300	(2.89±0.54)(12)			2
76 SLA/BLA3 ¹⁾ Vacuum-UV Photolysis.	EX	198-372	(6.93±1.81)(12)	0	569±70	2
¹⁾ k _a .						
71 LIN/KAU k _a + k _b .	EX	300	(2.11±0.72)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
$N(^2P) + N_2O \rightarrow N_2 + NO$						
Nitrogen atom + Nitrogen oxide (N_2O)						
72 HUS/KIR2	EX	300	(2.05±0.90)(12)			2
$N + HN_3 \rightarrow N_2 + N_2H$						
Nitrogen atom + Hydrazoic acid						
73 LEB/COM	EX	298	2.95(9)			2
$N + NH_2NH_2 \rightarrow NH + NH_2NH$ (a)						
$\rightarrow$ products (overall) (b)						
Nitrogen atom + Hydrazine						
75 YO	EX	298	2.7(10)			2
k_a .						
75 YO ¹⁾	EX	298-652	3.1(12)	0	1158	2
75 YO ¹⁾	EX	298	6.7(10)			2
¹⁾ k_b .						
$N + C (+ M) \rightarrow CN(B^2\Sigma^+) (+ M)$						
Nitrogen atom + Carbon atom						
75 WAS/KLE	EX	298	(3.41±0.91)(15)			3
M = Ar. Unreported T assumed to be 298 K.						
74 KLE/WAS	EX	298	3.41(15)			3
M = Ar. Resonance absorption.						
P(Total) = 1torr.						
$N(^2D) + CO_2 \rightarrow NO + CO$ (a)						
$\rightarrow N + O + CO$ (b)						
Nitrogen atom + Carbon dioxide						
71 LIN/KAU	EX	300	(3.01±1.20)(11)			2
$k_a + k_b$.						
$N + HCHO \rightarrow$ products						
Nitrogen atom + Formaldehyde						
71 WHI	EX	323-643	2.59(12)	0	1812±302	2
$N + CH_3OH \rightarrow HNO + CH_3$						
Nitrogen atom + Methanol						
73 ROS/ROS	EX	309-409	2.40(11)	0	4330±481	2 1.20
P = (1.07-1.56) torr.						
73 ROS/ROS	RL	299-306	(3.6±0.4)	0	0	2/2
k_{ref} : $N + CH_3OD \rightarrow$ products.						
73 ROS/ROS	RL	340-346	(8.0±1.0)	0	0	2/2
k_{ref} : $N + CD_3OD \rightarrow$ products.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
N + CH₃OD → DMO + CH₃						
Nitrogen atom + Methanol-d						
73 ROS/ROS ¹⁾ Average of 4 k's. P = (1.08-1.92) torr.	EX	299-306	(5.3±1.2)(7)	0	0	2
73 ROS/ROS ¹⁾ Average of 3 k's. P = (1.08-1.12) torr.	EX	340-346	(1.25±0.15)(8)	0	0	2
¹⁾ [CH ₃ OD] = (1.50-4.54) × 10 ¹⁸ molec.cm ⁻³ .						
N + CN → C + N₂						
Nitrogen atom + Cyanogen						
76 SLA	ES	5000-8000	(4.4±2.0)(14)	0	4529	2
N + CH≡CH → products						
Nitrogen atom + Ethyne						
77 MIC/LEE Discharge-flow. Resonance-fluorescence. Upper-limit k. P = (1.5-2.5) torr.	EX	298	<3.01(8)			2
79 SAT/SUG Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.	EX	300	(1.02±0.12)(10)			2
N + CH₂=CH₂ (+ M) → products						
Nitrogen atom + Ethene						
77 MIC/LEE Discharge-flow. Resonance-fluorescence. Upper-limit k. P = (1.5-2.5) torr. [N] ₀ ~ 1.0 × 10 ¹² molec.cm ⁻³ .	EX	298	<3.01(8)			2
79 ISH/SUG1 Pulse-radiolysis. Absorption-spectroscopy. Upper=limit k. P(Total) = (200-800) torr.	EX	298	≤3.98(10)			2
79 SAT/SUG Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.	EX	300	(3.91±0.78)(10)			2
80 HUS/SLA2 M = N ₂ . N ₂ O photolysis. Resonance-fluorescence.	EX	300	(3.41±0.22)(17)			3
N(²D) + CH₂=CH₂ → products						
Nitrogen atom + Ethene						
80 SUG/ISH2 Pulse-radiolysis. Resonance-absorption. P(Total) = (200-800) torr.	EX	298	(2.23±0.18)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
N(²P) + CH₂=CH₂ → products							
Nitrogen atom + Ethene							
80 SUG/ISH2 Pulse-radiolysis. Resonance-absorption. P(Total) = (200-700) torr.	EX	298	(1.69±0.12)(13)			2	
N + CH₃CH₂OH → HNO + CH₃CH₂							
Nitrogen atom + Ethanol							
73 ROS/ROS [CH ₃ CH ₂ OH] = (1.45-4.76)×10 ¹⁸ molec.cm ⁻³ . P = (1.12-1.63) torr.	EX	312-425	2.00(11)	0	4210±241	2	1.10
N + CH₃C≡CH → products							
Nitrogen atom + 1-Propyne							
77 MIC/LEE Discharge-flow. Resonance-fluorescence. Upper-limit k. P = (1.5-2.5) torr. [N] ₀ ~ 1.0×10 ¹² molec.cm ⁻³ .	EX	298	<3.01(8)			2	
N + CH₃CH=CH₂ → products							
Nitrogen atom + 1-Propene							
77 MIC/LEE Discharge-flow. Resonance-fluorescence. Upper-limit k. P = (1.5-2.5) torr. [N] ₀ ~ 1.0×10 ¹² molec.cm ⁻³ .	EX	298	<3.01(8)			2	
79 SAT/SUG Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.	EX	300	(6.63±1.20)(10)			2	
N + CH₃CH₂CH₂OH → HNO + CH₃CH₂CH₂							
Nitrogen atom + 1-Propanol							
73 ROS/ROS [CH ₃ CH ₂ OH] = (0.93-3.80)×10 ¹⁸ molec.cm ⁻³ . P = (1.29-1.48) torr.	EX	354-494	2.75(11)	0	3609±241	2	1.10
N + (CH₃)₂CHOH → HNO + (CH₃)₂CH							
Nitrogen atom + 2-Propanol							
73 ROS/ROS [CH ₃ CH ₂ OH] = (0.38-1.22)×10 ¹⁸ molec.cm ⁻³ . P = (0.865-1.73) torr.	EX	304-449	8.51(11)	0	4691±241	2	1.12

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
N + CH₂=CHCH=CH₂ → products						
Nitrogen atom + 1,3-Butadiene						
79 SAT/SUG Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.	EX	300	(6.63±0.60)(10)			2
N + CH₃CH₂CH=CH₂ → products						
Nitrogen atom + 1-Butene						
79 SAT/SUG Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.	EX	300	(6.63±0.60)(10)			2
N + cis-CH₃CH=CHCH₃ → products						
Nitrogen atom + 2-Butene, (Z)-						
79 SAT/SUG Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.	EX	300	(3.91±0.48)(10)			2
N + trans-CH₃CH=CHCH₃ → products						
Nitrogen atom + 2-Butene, (E)-						
79 SAT/SUG Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.	EX	300	(4.04±0.54)(10)			2
N + (CH₃)₂C=CH₂ → products						
Nitrogen atom + 1-Propene, 2-methyl-						
79 ISH/SUG1 Pulse-radiolysis. Absorption-spectroscopy. Upper-limit k. P(Total) = (200-600) torr.	EX	298	≤8.43(10)			2
79 SAT/SUG Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.	EX	300	(1.08±0.12)(11)			2
N + NCC=CCN → [N.C₄N₂[†]]						
Nitrogen atom + 2-Butynedinitrile (Dicyanoacetylene)						
72 HAN/OBE2	ES	300	(3.19±2.59)(9)			2
N + (CH₃)₂C=CHCH₃ → products						
Nitrogen atom + 2-Butene, 2-methyl-						
79 SAT/SUG Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.	EX	300	(4.94±0.48)(10)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
N₂ (+ M) → N + N (+ M)						
Nitrogen molecule						
74 KEW/HOR ¹⁾ M = N.	EX	6000-14000	5.54(19)	-2.5	113200	2 1.58
74 KEW/HOR ¹⁾ M = N ₂ .	EX	6000-14000	5.03(20)	-3.5	113200	2 1.58
¹⁾ The preexponential factor expressed as: A(T/298) ⁿ .						
N₂(A³Σ_u⁺) + O₂ → N₂(X¹Σ) + O₂[*] (a)						
→ N ₂ (X ¹ Σ) + O(¹ P) + O(¹ P) (b)						
→ N ₂ O(X ² Π) + O(³ P) (c)						
→ N ₂ O(X ² Π) + O(¹ D) (d)						
Nitrogen molecule + Oxygen molecule						
82 IAN/JEF ¹⁾ k _a .	ES	298	≈6.02(11)			2
82 IAN/JEF ¹⁾ k _b .	ES	298	≈1.20(12)			2
82 IAN/JEF ¹⁾ k _c + k _d .	ES	298	≈3.61(10)			2
82 IAN/JEF ¹⁾ k _a + k _b + k _c + k _d .	EX	298	1.81(12)			2
¹⁾ M = Ar. Discharge-flow. Laser-induced fluorescence. Weighted average k's. P(Total) ~ 2 torr.						
N₂(A³Σ_u⁺, v=n) + O₂ → products						
Nitrogen molecule + Oxygen molecule						
81 IAN/KAU ¹⁾ n = 0.	EX	298	(1.51±0.24)(12)			2
81 IAN/KAU ¹⁾ n = 1.	EX	298	(2.35±0.36)(12)			2
81 IAN/KAU ¹⁾ n = 2.	EX	298	(2.59±0.42)(12)			2
¹⁾ Discharge-flow. Laser-induced fluorescence.						
N₃ + N₃ → N₂ + N₂ + N₂						
Azide						
79 JOU/LEB1 Calculation based on computer simulation.	DE	298	(3.91±0.90)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
NO (+ M) → N + O (+ M)							
Nitrogen oxide (NO)							
73 MYE M = Ar.	EX	2600-6300	1.37(14)	0	74685	2	
73 MYE M = NO. Upper-limit estimate.	ES	2600-6300	≤3.0(14)	0	76497	2	
NO + O₂(¹Δ_g) → NO₂ + O							
Nitrogen oxide (NO) + Oxygen molecule							
76 DUM	EX	298	2.94(6)			2	
NO + NO → N₂ + O₂ (a) → N₂O + O (b)							
Nitrogen oxide (NO)							
75 TRU/MAC k _a . M = Ne. The preexponential factor expressed as: A(T/298) ^{0.5} .	EX	2700-4700	3.07(12)	0.5	30458	2	
73 MYE k _b .	EX	2595-6300	2.35(10)	0	14595	2	
76 MCC/KRU k _b . Best fit to the experimental data.	EX	1750-2100	1.80(12)	0	32109	2	2.04
77 MCC/KRU k _b . Flow reactor.	EX	1750-2100	1.80(12)	0	32109	2	2.0
79 KOS/ASA k _b . Incident shock-waves. Computer simulation. [NO] = (2.4-4.2) × 10 ¹⁸ molec.cm ⁻³ . P _O = 30 torr.	DE	2700-3500	4.9(12)	0	33770	2	
NO + NO + NO → NO₂ + N₂O							
Nitrogen oxide (NO)							
79 GVO/NES1 ¹) P = (6.0- 10.5) torr.	EX	753-813	1.26(10)	0	13589±1007	3	2.88
79 GVO/NES2 ¹) P = (22.5-112.5) torr.	EX	713-923	1.07(10)	0	13488±151	3	1.15
¹) NO oxidation in a stainless-steel vessel.							
NO + NO + O₂ → NO₂ + NO₂							
Nitrogen oxide (NO) + Oxygen molecule							
73 STE/NIK1	EX	298	(1.45±0.07)(10)			3	
75 ENG/COR	EX	298	(1.46±0.03)(10)			3	
75 ENG/COR	EX	298-323	(1.99±0.28)(9)	0	-591±43	3	
A and B recalculated from the reported data.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
NO + NO₂ + H₂O → HONO + HONO							
Nitrogen oxide (NO) + Nitrogen oxide (NO ₂) + Water							
75 ENG/COR Best data-fit by optimization.	ES	298-323	(1.5±0.5)(11)	0	0	3	
76 CHA/NOR k ₁ = Kk ₋₁ .	DE	296	(2.19±0.70)(10)			3	
NO + NO₃ → NO₂ + NO₂							
Nitrogen oxide (NO) + Nitrogen oxide (NO ₂)							
73 HAR/JOH	RN	296	5.24(12)			2	
74 GLA/TRO1 Best fit to the experimental data.	ES	1000-1100	(8.0±4.0)(12)			2	
75 GRA k ₁ = Kk ₋₁ .	DE	297	(1.13±0.25)(13)			2	
78 GRA/JOH Modulated photolysis technique. k ₁ = k ₋₁ K.	DE	297	(1.14±0.24)(13)			2	
NO + N₂O → NO₂ + N₂							
Nitrogen oxide (NO) + Nitrogen oxide (N ₂ O)							
73 BOR/SKA	ES	1050-2510	2.75(14)	0	25164±1510	2	1.58
79 GVO/NES3 N ₂ O decomposition in a stainless-steel vessel under static conditions. Gas-chromatography. P = (22.5-112.5) torr.	EX	713-923	1.51(11)	0	24811±302	2	2.51
NO + NH₂ → N₂ + H₂O							
Nitrogen oxide (NO) + Amidogen							
71 GOR/MUL Unreported T assumed to be 298 K.	EX	298	1.6(13)			2	
72 BED/THO k _{ref} : NH ₂ + NO ₂ → NH + HONO.	RL	615-660	5.01(-3)	0	-3221±503	2/2	
73 GEH/HOY The water molecule formed as product is vibrationally excited.	EX	298	(5.0±1.0)(12)			2	
NO + NH₃ → HNO + NH₂							
Nitrogen oxide (NO) + Ammonia							
78 ROO/HAN Shock-waves.	ES	1700-3000	5.0(14)	0	25164	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units factor	k err.
NO + HNO → products							
Nitrogen oxide (NO) + Nitrosyl hydride							
81 CHE/NAD CH ₃ CHO/NO flash-photolysis. P(HCHO) = 7 torr. P(CH ₃ CHO) = 12.2 torr. P(NO) = (20-380) torr.	EX	298	(3.01±0.90)(5)				2
NO + HONO₂ → NO₂ + HONO							
Nitrogen oxide (NO) + Nitric acid							
77 KAI/WU	EX	300	9.03(3)				2
79 MCK/MAT Flow-reactor. Spectrophotometry. P = 760 torr.	EX	298	8.4(3)				2
79 STR/WEL Tunable diode-laser. Static reactor.	EX	296	(2.05±1.20)(2)				2
NO + C₂O → NCO + CO (a) → CNO + CO (b)							
Nitrogen oxide (NO) + Carbon oxide (C ₂ O)							
80 DON/PIT k _a + k _b . Laser photodissociation of C ₃ O ₂ nm. Dye-laser induced fluorescence.	EX	298	(2.61±0.07)(13)				2
NO₂ (+ M) → NO + O (+ M)							
Nitrogen oxide (NO ₂)							
79 END/GLA M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.61(Ar), 0.61(Kr), 0.69(Xe), 0.82(Ne), 2.04(CO ₂), 2.04(CF ₄), 2.14(He). Thermolysis in shock-waves. Rate constants expressed as k[M].	EX	1800	2.45(8)				2
NO₂ + NO₂ → NO + NO₃ (a) → NO + anti-NO₃ (b)							
Nitrogen oxide (NO ₂)							
73 BUT/LEV k _a .	ES	1700-2400	(3.2±1.0)(12)	0	12870		2
77 FRE/PAL k _b .	ES	1471-1855	3.16(13)	0	17111		2
NO₂ + NO₂ + CH₃OH → HONO₂ + CH₃ONO							
Nitrogen oxide (NO ₂) + Methanol							
82 NIK/MAK1 FTIR-spectroscopy. P(CH ₃ OH) = (0-1.0) torr. P(NO ₂) = (0-1.0) torr. P(N ₂) = 700 torr.	EX	298	(2.07±0.22)(11)				3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{NO}_2 + \text{NO}_2 + \triangle \rightarrow \text{products}$						
Nitrogen oxide (NO_2) + Oxirane						
71 JAF Preliminary results.	EX	298-373	1.3(12)	0	1862	3
$\text{NO}_2 + \text{NO}_2 + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{HONO}_2 + \text{CH}_3\text{CH}_2\text{ONO}$						
Nitrogen oxide (NO_2) + Ethanol						
82 NIK/MAK1 FTIR-spectrometry. $P(\text{CH}_3\text{CH}_2\text{OH}) = (0.1-1.0)$ torr. $P(\text{NO}_2) = (0-1.0)$ torr. $P(\text{N}_2) = 700$ torr.	EX	298	(2.07±0.29)(11)			3
$\text{NO}_2 + \text{NO}_3 (+\text{M}) \rightarrow \text{NO} + \text{NO}_2 + \text{O}_2 (+\text{M})$ (a) $\rightarrow \text{N}_2\text{O}_5 (+\text{M})$ (b)						
Nitrogen oxide (NO_2) + Nitrogen oxide (NO_3)						
75 GRA $k_a. k_a = k_{-a}K.$	DE	298-329	(1.51±0.30)(10)	0	1228±101	2
78 GRA/JOH k_a . Modulated photolysis. $k_a = k_{-a}K.$	DE	298-329	(1.51±0.30)(10)	0	1230±100	2
80 CON k_b . $M = \text{N}_2$. Limiting high-pressure k. $\text{N}_2\text{O}_5/\text{NO}$ thermolysis. $[\text{N}_2] < 2 \times 10^{18}$ molec.cm ⁻³ .	EX	262-272	1.28(14)	0	1360	2
82 FOW/MIT k_b . Closed system. NO_3 generated by injecting NO_2 in a O_3 flow. k expressed as k[M]. $[\text{NO}_2]_0 = (0.1-1.0) \times 10^{13}$ molec.cm ⁻³ . $[\text{O}_3] = (5.5-7.4) \times 10^{17}$ molec.cm ⁻³ .	EX	298	(1.20±0.48)(12)			2
82 MAL/TRO k_b . Limiting high-pressure k. Recommended k, in terms of unimolecular rate theory. The pre- exponential factor expressed as: $A(T/298)^{0.2}$.	RE	200-300	9.62(11)	0.2	0	2
80 CON k_b . $M = \text{N}_2$. Limiting low-pressure k. $\text{N}_2\text{O}_5/\text{NO}$ Thermolysis. 10^{18} molec.cm ⁻³ .	EX	268-307	3.48(15)	0	-1550	3
78 WAY/MIT k_b . Flow-reactor. $M = \text{NO}_2, \text{O}_2$. Preliminary k.	ES	298	1.31(16)			3
82 MAL/TRO k_b . Rate constant expressed as k/[M]. Limiting low-pressure k. Recommended k, evaluated in terms of unimolecular rate theory. The pre- exponential factor expressed as $A(T/298)^{-4.1}$.	RE	200-300	1.38(18)	-4.1	0	3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{NO}_2 + \text{NH}_3 \rightarrow \text{HONO} + \text{NH}_2$						
Nitrogen oxide (NO_2) + Ammonia						
72 BED/THO Cylindrical Pyrex reaction vessel. Photomultiplier. Logarithmic amplifier.	EX	615-660	3.98(12)	0	13916±51	2 2.0
$\text{NO}_2 + \text{HONO} \rightarrow \text{NO} + \text{HONO}_2$						
Nitrogen oxide (NO_2) + Nitrous acid						
79 STR/WEL Tunable diode-laser. Static reactor. $k_1 = k_{-1}K$.	DE	296	≤6.02(1)			2
$\text{NO}_2 + \text{CH}_4 \rightarrow \text{HONO} + \text{CH}_3$						
Nitrogen oxide (NO_2) + Methane						
78 SLA/GRI3 Shock-waves. P = (2-4) Atm.	ES	1300-1900	7.0(11)	0	15098	2
81 SLA/GRI $\text{CH}_4/\text{O}_2/\text{Ar}$ ignition sensitized by NO_2 behind reflected shock-waves. P = (1.8-3.6) atm.	ES	1310-1790	1.2(13)	0	15098	2
$\text{NO}_2 + \text{HCN} \rightarrow \text{HONO} + \text{CN}$ (a) $\rightarrow \text{HNO} + \text{NCO}$ (b)						
Nitrogen oxide (NO_2) + Hydrocyanic acid						
82 FIF/HOL ¹⁾	EX	1300	≤1.0(7)			2
82 FIF/HOL ¹⁾	EX	1800	≤1.0(10)			2
¹⁾ $k_a = k_b$. Reaction behind shock-waves in Ar. Upper-limit k's. P = (1.7-12.6) atm.						
$\text{NO}_2 + \text{CH}_2=\text{CH}_2 \rightarrow \text{products}$						
Nitrogen oxide (NO_2) + Ethene						
71 JAF	EX	298-373	2.00(6)	0	4145	2
71 JAF	EX	298	1.82			2
$\text{NO}_2 + \text{CH}_3\text{CHO} \rightarrow \text{HONO} + \text{CH}_3\text{CO}$						
Nitrogen oxide (NO_2) + Acetaldehyde						
71 JAF	EX	298-373	1.58(5)	0	3473	2
71 JAF	EX	298	1.50			2
72 DAV/COR	EX	295	(8.596±0.189)			2
72 DAV/COR The A-factor recalculated from the reported experimental data.	EX	295-395	3.10(10)	0	6492±302	2
74 JAF/WAN	EX	295-390	2.51(10)	0	6241	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
NO₂ + CH₃C≡CH → products						
Nitrogen oxide (NO ₂) + 1-Propyne						
73 ASH/THO	EX	443-493	4.68(8)	0	6427±81	2 1.20
NO₂ + CH₃CH=CH₂ → products						
Nitrogen oxide (NO ₂) + 1-Propene						
71 JAF	EX	298-373	3.2(6)	0	3914	2
71 JAF	EX	298	6.24			2
76 GRY/ROZ	EX	293-373	2.4(5)	0	2818	2
NO₂ + CH₃CH₂CH₃ → HONO + (CH₃)₂CH						
Nitrogen oxide (NO ₂) + Propane						
76 TIT/BAL	EX	423-498	2.40(11)	0	11374±60	2 1.12
NO₂ + CH₃CH₂CHO → HONO + CH₃CH₂CO						
Nitrogen oxide (NO ₂) + Propanal						
74 JAF/WAN	EX	295-390	2.51(10)	0	6241	2
NO₂ + (CH₃)₂CO → HONO + CH₃COCH₃						
Nitrogen oxide (NO ₂) + 2-Propanone						
71 JAF	EX	298-373	3.8(5)	0	3588	2
71 JAF	EX	298	2.4			2
NO₂ + CH₂=CHC≡CH → products						
Nitrogen oxide (NO ₂) + 1-Buten-3-yne						
75 GRY/ROZ	EX	273-333	8.8(5)	0	1711	2
NO₂ + CH₃C≡CCH₃ → products						
Nitrogen oxide (NO ₂) + 2-Butyne						
73 ASH/THO	EX	443-493	3.63(8)	0	6029±96	2 1.23
NO₂ + CH₃CH₂CH=CH₂ → products						
Nitrogen oxide (NO ₂) + 1-Butene						
71 JAF	EX	298-373	2.51(6)	0	3684	2
71 JAF	EX	298	1.07(1)			2
NO₂ + cis-CH₃CH=CHCH₃ → products						
Nitrogen oxide (NO ₂) + 2-Butene, (Z)-						
71 JAF	EX	298-373	2.51(5)	0	2763	2
71 JAF	EX	298	2.36(1)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
NO₂ + trans-CH₃CH=CHCH₃ → products						
Nitrogen oxide (NO ₂) + 2-Butene, (E)-						
71 JAF	EX	298-373	1.58(6)	0	3224	2
71 JAF	EX	298	3.17(1)			2
NO₂ + (CH₃)₂C=CH₂ → products						
Nitrogen oxide (NO ₂) + 1-Propene, 2-methyl-						
71 JAF	EX	298-373	3.98(4)	0	1980	2
71 JAF	EX	298	5.17(1)			2
NO₂ + CH₃CH₂CH₂CHO → HONO + CH₃CH₂CH₂CO						
Nitrogen oxide (NO ₂) + Butanal						
74 JAF/WAN	EX	295-390	2.51(10)	0	6241	2
NO₂ + CH₃CH₂N(1O)=CHCH₃ → NO + CH₃CH₂NO + CH₃CHO						
Nitrogen oxide (NO ₂) + Ethanamine, N-ethylidene- N-oxide						
82 GLE/HEI ¹⁾ Lower-limit k.	EX	298	>6.02(7)			2
82 GLE/HEI ¹⁾ k _{ref} : (CH ₃ CH ₂) ₂ NO + CH ₃ CH ₂ N(1O)=CHCH ₃ → adduct	RL	298	3.0(-1)			2/2
¹⁾ Diethylhydroxylamine oxidation by NO ₂ in a IR gas-cell. [NO ₂] (15-236) mtorr. [HONO] = (11-15) mtorr. [(CH ₃ CH ₂) ₂ NOH] = (25-45) mtorr.						
NO₂ + (CH₃CH₂)₂NOH → HONO + (CH₃CH₂)₂NO (a) → any other products (b)						
Nitrogen oxide (NO ₂) + Ethanamine, N-ethyl-N-hydroxy-						
82 GLE/HEI k _a . Diethylhydroxylamine oxidation by NO ₂ in a IR gas-cell. [NO ₂] (15-236) mtorr. [HONO] = (11-15) mtorr. [(CH ₃ CH ₂) ₂ NOH] = (25-45) mtorr.	ES	298	(3.31±0.60)(6)			2
74 JAY/SIM k _{overall} . Dark reaction of (CH ₃ CH ₂) ₂ NOH (diluted in CO ₂) with NO ₂ (diluted in O ₂). High-vacuum. P(Diethylhydroxylamine) = 2.2 mtorr. P(NO ₂) = 19.3 mtorr.	EX	298	2.71(6)			2
NO₂ + CH₂=CHC(CH₃)=CH₂ → products						
Nitrogen oxide (NO ₂) + 1,3-Butadiene, 2-methyl-						
75 GRY/ROZ	EX	273-433	1.7(7)	0	1056	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units factor	k err.
NO₂ + CH₃CH₂CH₂CH=CH₂ → products							
Nitrogen oxide (NO ₂) + 1-Pentene							
71 JAF	EX	298-373	1.58(6)	0	3684	2	
71 JAF	EX	298	6.76			2	
NO₃ + NO₃ → NO₂ + NO₂ + O₂							
Nitrogen oxide (NO ₃)							
75 GRA	EX	298-329	(5.12±1.69)(11)	0	2451±101	2	
78 GRA/JOH	EX	298-329	(5.12±1.69)(11)	0	2450±100	2	
Modulated photolysis.							
80 AFA/DOR	CO	300-350	(1.69±0.24)(12)	0	3400±600	2	
Given with caution.							
Indirect measurement based on the literature							
data for the reaction:							
$\text{NO}_2 + \text{O}_3 \rightarrow \text{NO}_3 + \text{O}_2$							
and K for reaction:							
$\text{N}_2\text{O}_5 = \text{NO}_2 + \text{NO}_3$.							
NO₃ + CH₂=CH₂ → products							
Nitrogen oxide (NO ₃) + Ethene							
75 JAF/NIK	EX	300	(5.60±0.60)(8)			2	
Data fit to a proposed mechanism.							
NO₃ + CH₃CHO → HONO₂ + CH₃CO							
Nitrogen oxide (NO ₃) + Acetaldehyde							
74 MOR/NIK	EX	300	7.23(8)			2	1.25
Best fit of experimental data.							
NO₃ + CH₃CH=CH₂ → products							
Nitrogen oxide (NO ₃) + 1-Propene							
75 JAF/NIK	EX	300	(3.19±0.18)(9)			2	
Data fit to a proposed mechanism.							
NO₃ + CD₃CD=CD₂ → products							
Nitrogen oxide (NO ₃) + 1-Propene-d ₆							
75 JAF/NIK	EX	300	(3.55±0.24)(9)			2	
Data fit to a proposed mechanism.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
NO₃ + CH₃CH₂CH=CH₂ → products						
Nitrogen oxide (NO ₃) + 1-Butene						
75 JAP/NIK	EX	300	(4.69±0.48)(9)			2
Data fit to a proposed mechanism.						
NO₃ + cis-CH₃CH=CHCH₃ → products						
Nitrogen oxide (NO ₃) + 2-Butene, (Z)-						
75 JAP/NIK	EX	300	(1.08±0.12)(11)			2
Data fit to a proposed mechanism.						
NO₃ + trans-CH₃CH=CHCH₃ → products						
Nitrogen oxide (NO ₃) + 2-Butene, (E)-						
75 JAP/NIK	EX	300	(8.43±0.60)(10)			2
Data fit to a proposed mechanism.						
NO₃ + (CH₃)₂C=CH₂ → products						
Nitrogen oxide (NO ₃) + 1-Propene, 2-methyl-						
75 JAP/NIK	EX	300	(6.63±0.60)(10)			2
Data fit to a proposed mechanism.						
NO₃ + CH₃CH=C(CH₃)₂ → products						
Nitrogen oxide (NO ₃) + 2-Butene, 2-methyl-						
75 JAP/NIK	EX	300	(3.31±0.30)(12)			2
Data fit to a proposed mechanism.						
NO₃ + (CH₃)₂C=C(CH₃)₂ → products						
Nitrogen oxide (NO ₃) + 2-Butene, 2,3-dimethyl-						
75 JAP/NIK	EX	300	(2.23±0.30)(13)			2
Data fit to a proposed mechanism.						
N₂O (+ M) → N₂ + O (+ M) (a)						
→ any other products (b)						
Nitrogen oxide (N ₂ O)						
71 D'A	EX	1600-2500	2.88(1)	0	27680	2
k _a . M = Ar.						
Rate constant expressed as: k/[M].						
71 LIP	EX	1400-2000	1.35(13)	0	24555±2235	2 3.98
k _a . M = Kr.						
72 BOR/SKA	EX	1000-2000	5.01(14)	0	28686±755	2 2.0
k _a . M = Ar + N ₂ .						
Reflected shock-waves.						
72 SOL	SE	1000-3000	4.7(14)	0	29190	2
k _a . M = N ₂ O.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
72 VER/KIS k _a . M = N ₂ . Limiting high-pressure k.	EX	1250-1800	1.4(11)	0	26573	1	
73 LIP/MIL k _a . M = Kr.	EX	1300-1950	1.26(13)	0	22194	2	
75 BAB/DEA k _a . M = Ar.	EX	1850-2535	7.83(14)	0	28628	2	
75 DOV/NIP k _a . M = Ar.	EX	2160-2500	5.01(13)	0	29190	2	
76 DEA k _a . Data fit to a proposed mechanism.	ES	1950-3075	1.96(14)	0	25861	2	
77 BAL/VAN k _a . M = H ₂ . Supersonic molecular beam. Mass-spectrometry. P = 40 torr.	EX	1670-1980	(1.3±0.4)(15)	0	28435	2	
77 DEA/STE1 k _a . M = Ar. Shock-waves. N ₂ O/CO/Ar mixtures at a total concentration of (2.5-7.7)×10 ¹⁸ molec.cm ⁻³ .	EX	2100-3200	2.71(14)	0	27184	2	
77 MON/HAN1 k _a . M = Ar, Kr, N ₂ , or O ₂ . Best data-fit.	ES	1815-3365	1.42(14)	0	25808	2	1.5
79 END/GLA k _a . M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.52(Xe), 0.61(Kr), 0.78(Ar), 1.48(Ne), 4.26(He), 4.81(CF ₄). Thermolysis in shock-waves. Rate constants expressed as k[M].	EX	2000	2.7(8)			2	
80 SUL/KLI k _a . M = Ar. Thermolysis behind shock-waves. P = (1300-3500) torr.	EX	1685-2560	(3.71±2.74)(14)	0	13920±727	2	
80 ZAS/LOS k _a . M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 2.0(N ₂), 3.0(CO), 4.0(He). [Ar] = (0.6-1.4)×10 ¹⁹ molec.cm ⁻³ . Thermolysis of N ₂ in Ar, He, N ₂ , or CO, behind shock-waves.	EX	1700-2500	4.4(14)	0	28183	2	
71 LIP k _{overall} . M = Kr.	EX	1400-2000	3.09(12)	0	20493±1550	2	3.98
73 VOM2 k _{overall} . M = Ne. Low-pressure k.	EX	1800-2400	3.16(13)	0	21641±2013	2	2.51
74 TRA ¹) k _{overall} . Shock-tube. Unspecified high-T range.	EX	¹)	3.63(14)	0	26724	2	
75 BAB/DEA k _{overall} .	EX	1850-2525	2.95(14)	0	26355±625	2	1.32
76 DEA ²) Without added H ₂ .	EX	1950-3075	1.15(14)	0	24478±433	2	1.20

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
76 DEA ²⁾ With 0.01% H ₂ added. ²⁾ k _{overall} .	EX	1950-3075	5.25(13)	0	22072±433	2	1.20
N₂O₅ (+ M) → NO₂ + NO₃ (+ M) (a) → any other products (b)							
Nitrogen oxide (N ₂ O ₅)							
79 CON/JOH ¹⁾ k _a . M = N ₂ . Limiting high-pressure k.	EX	262-345	1.78(17)	0	12540±130	1	
80 CON ²⁾ k _a . M = N ₂ . Limiting high-pressure k.	EX	268-307	1.78(17)	0	12540±200	1	
81 VIG/DAV ²⁾ k _a . Troe fit. Limiting high-pressure k.	RE	285-384	1.21(17)	0	12662±322	1	
81 VIG/DAV ³⁾ k _a . Johnston fit. Limiting high-pressure k.	EX	285-384	1.8(17)	0	12788±242	1	
82 FOW/MIT k _a . M = O ₂ . NO ₃ generated by injecting NO ₂ in a O ₃ flow. k expressed as k[M]. [O ₂] = (2.7-5.1)×10 ¹⁸ molec.cm ⁻³ . [NO ₂] ₀ > 1.0×10 ¹⁴ molec.cm ⁻³ .	EX	298	(1.0±0.6)(-1)			1	
82 MAL/TRO ⁴⁾ k _a . M = N ₂ . Limiting high-pressure k.	TH	220-300	9.69(14)	0.1	11080	1	
79 CON/JOH ¹⁾ k _a . M = N ₂ . Limiting low-pressure k. ¹⁾ quartz reactor. IR-Spectrometry.	EX	262-345	3.67(18)	0	9570±200	2	
80 CON ²⁾ k _a . M = N ₂ . Limiting low-pressure k. ²⁾ N ₂ O ₅ Thermolysis in presence of NO. [N ₂] < 2×10 ¹⁸ molec.cm ⁻³ .	EX	268-307	4.85(18)	0	9630±200	2	
81 VIG/DAV ³⁾ k _a . Troe fit. Limiting low-pressure k.	RE	285-384	6.93(18)	0	9914±453	2	
81 VIG/DAV ³⁾ k _a . Johnston fit. Limiting low-pressure k. ³⁾ Flowing-afterglow. Mass-spectrometry. Data-fit to theoretical models. P = (10-800) torr.	EX	285-384	3.28(18)	0	9653±292	2	
82 MAL/TRO ⁴⁾ k _a . M = N ₂ . Rate constant expressed as k/[M]. Limiting-low-pressure k. ⁴⁾ Critical evaluations. The preexponential factor expressed as: A(T/298) ⁿ .	TH	220-300	1.36(21)	-4.4	11080	2	
72 DUT/BUN k _{overall} . Preliminary rate constant.	EX	308	(1.11±0.21)(-4)			1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
NH + O₂ → NO + OH (a)						
→ NO ₂ + H (b)						
→ HNO + O (c)						
Imidogen + Oxygen molecule						
79 PAG/ERI k _a . Gaseous NH ₃ pulse-radiolysis. Upper-limit k.	ES	300	≤2.0(10)			2
78 ZET/HAN k _a + k _b + k _c . Resonance-fluorescence. UV-photo- lysis. Channel (c) is the most probable path.	EX	296	(5.12±0.54)(9)			2
NH + H₂ → NH₂ + H						
Imidogen + Hydrogen molecule						
79 DOV/NIP ¹⁾	EX	2601	1.8(12)			2
79 DOV/NIP ¹⁾	EX	2788	2.2(12)			2
¹⁾ Pyrolysis behind reflected shock-waves.						
NH + N₂ (+ M) → HN₃ (+ M) (a)						
→ any other products (b)						
Imidogen + Nitrogen molecule						
81 ZET/STU k _a . M = N ₂ . Pulsed vacuum-UV photolysis of NH ₃ at 105 nm. Resonance-fluorescence. Upper-limit k. P(NH ₃) = (0.005-0.9) torr. P(N ₂) < 900 torr.	EX	298	<3.63(9)			3
81 ZET/STU k _{overall} . Pulsed vacuum-UV photolysis of NH ₂ at 105 nm. Resonance-fluorescence. Upper-limit k. P(NH ₃) = (0.005-0.9) torr.	EX	298	<1.81(5)			2
NH + NO → H + N₂O (a)						
→ any other products (b)						
Imidogen + Nitrogen oxide (NO)						
78 ROO/HAN ¹⁾ k _a . Shock-waves. The preexponential factor expressed as: A(T/298) ^{0.75} .	ES	1700-3000	6.46(11)	0.75	0	2
81 ROO/HAN ¹⁾ k _a . Best data-fit. ¹⁾ NH ₃ /NO, or N ₂ O in Ar behind incident shock-waves. Emission and IR-laser Absorption.	EX	1760-2850	8.0(13)	0	14800	2 3.0
71 GOR/MUL k _{overall} . Unreported T assumed to be 298 K.	EX	298	2.3(13)			2
76 HAN/HOE k _{overall} . Unreported T assumed to be 298 K.	EX	298	(2.83±0.72)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 MOR2 k _{overall} . Premixed H ₂ /O ₂ /Ar Flames. Laser-Fluorescence. Upper-limit k. P = 760 torr.	EX	1790	<4.22(12)			2
NH + NH ₂ → NH ₂ NH Imidogen + Amidogen						
79 PAG/ERI Gaseous NH ₃ pulse-radiolysis.	EX	349	7.0(13)			2
NH + NH ₃ (+ M) → NH ₂ NH ₂ (+ M) (a) → any other products (b) Imidogen + Ammonia						
81 ZET/STU ¹) k _a . M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.06(He) 1.00(Ar), 60.22(NH ₃). P(M) <900 torr.	EX	298	<1.8(13)			3
81 ZET/STU ¹) k _{overall} . ¹) Pulsed vacuum-UV Photolysis of NH ₃ at 105 nm. Resonance-fluorescence. P(NH ₃) = (0.05-0.9) torr.	EX	298	<4.82(7)			2
NH(a ¹ Δ) + HN ₃ (¹ A') → NH ₂ (² A ₁) + N ₃ (² Π _g) (a) → NH(X ³ Σ ⁻) + NH(X ³ Σ ⁻) + N ₂ (X ¹ Σ) (b) Imidogen + Hydrazoic acid						
73 PAU/BAI k _a + k _b . Unreported T assumed to be 298 K.	EX	298	(1.51±0.60)(13)			2
76 PAU/BAI k _a . Upward revised k.	EX	298	(5.60±0.60)(13)			2
78 MCD/MIL k _a . HN ₃ photolysis. Gas-chromatography.	EX	298	(5.60±0.54)(13)			2
80 PIP/KRE k _a . UV-photolysis of HN ₃ at 290 nm. Laser-induced fluorescence. P(Total) = (5-50) torr.	EX	298	1.08(14)			2
NH(b ¹ Σ ⁺) + NH ₃ → products Imidogen + Ammonia						
75 ZET/STU	EX	298	2.46(11)			2 1.25

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{NH}(a^1\Delta) + \text{CH}_4 \rightarrow \text{NH}_2(^2A_1) + \text{CH}_3$ (a) $\quad \quad \quad \rightarrow \text{NH}_2(^2B_1) + \text{CH}_3$ (b) $\quad \quad \quad \rightarrow \text{NH}_2\text{CH}_3$ (c)						
Imidogen + Methane						
78 MCD/MIL	EX	298	(7.23±0.60)(12)			2
$k_a + k_b + k_c$. HN_3 photolysis. Gas-chromatography. Channel (c) is favored.						
$\text{NH}(a^1\Delta) + \text{CH}_2=\text{CH}_2 \rightarrow \text{NH}_2(^2A_1) + \text{CH}_2=\text{CH}$ (a) $\quad \quad \quad \rightarrow \text{NH}_2(^2B_1) + \text{CH}_2=\text{CH}$ (b) $\quad \quad \quad \rightarrow \text{NH} \begin{array}{c} \text{H} \\ \diagup \quad \diagdown \\ \text{N} \end{array}$ (c)						
Imidogen + Ethene						
78 MCD/MIL	EX	298	(2.29±0.24)(13)			2
$k_a + k_b + k_c$. HN_3 photolysis. Gas-chromatography. Channel (c) is favored.						
$\text{NH}(a^1\Delta) + \triangle \rightarrow \text{NH}_2(^2A_1) + \triangle^\bullet$ (a) $\quad \quad \quad \rightarrow \text{NH}_2(^2B_1) + \triangle^\bullet$ (b)						
Imidogen + Cyclopropane						
78 MCD/MIL	EX	298	(2.17±0.54)(13)			2
$k_a + k_b$. HN_3 photolysis. Gas-chromatography.						
$\text{NH}(a^1\Delta) + \text{Cyclohexane} \rightarrow \text{NH}_2(^2A_1) + \text{Cyclohexyl}^\bullet$ (a) $\quad \quad \quad \rightarrow \text{NH}_2(^2B_1) + \text{Cyclohexyl}^\bullet$ (b)						
Imidogen + Cyclohexane						
78 MCD/MIL	EX	298	(4.03±0.42)(13)			2
$k_a + k_b$. HN_3 photolysis. Gas-chromatography.						
$\text{NH}_2 + \text{O}_2 (+\text{M}) \rightarrow \text{NH}_2\text{O}_2 (+\text{M})$ (a) $\quad \quad \quad \rightarrow \text{HNO} + \text{OH} (+\text{M})$ (b) $\quad \quad \quad \rightarrow \text{NO} + \text{H}_2\text{O} (+\text{M})$ (c)						
Amidogen + Oxygen molecule						
79 PAG/ERI	ES	300	≤5.0(9)			2
$k_a = k_b = k_c$. Gaseous NH_3 pulse-radiolysis. Upper-limit k's.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 FUJ/MIY1 k _a . Oxidation of NH ₃ behind reflected shock-waves. The product is vibrationally excited.	DE	300-1200	3.16(12)	0	7549±252	2
79 FUJ/MIY k _b . Shock-wave induced high-T oxidation of NH ₃ . Computer simulation based on a reaction scheme including 13 steps, under the following conditions: [NH ₃] = [O ₂] = 5%. [Ar] = 90%, and P = (3.7-7.7) atm.	DE	1492-2319	1.26(13)	0	14092	2
77 LES/DEM k _a + k _b + k _c . NH ₃ flash-photolysis. P(NH ₃) = 3 torr. Upper-limit k.	EX	298-500	≤1.81(6)			2
79 CHE/SAR k _a + k _b + k _c . NH ₃ Flash-photolysis. Laser-Spectroscopy. Upper-limit k. P < 570 torr.	EX	298	<9.03(6)			2
79 NAD/SAR4 k _a + k _b + k _c . Laser spectroscopy. Upper-limit k.	EX	298	<4.82(7)			2
82 HAC/HOR k _a . M = He. Discharge flow. Laser-induced fluorescence. P = (1.5-16) torr. Limiting low-pressure k. The preexponential factor expressed as: A(T/298) ^{-2.0} .	EX	295-353	(1.27±0.50)(15)	-2.0	0	3
NH ₂ + O ₃ → HONO + OH (a) → HNO + HO ₂ (b) → NH ₂ O + O ₂ (c)						
Amidogen + Ozone						
80 HAC/HOR k _a + k _b + k _c . Discharge-flow. NH ₃ + F → NH ₂ + HF.	EX	250-360	1.28(12)	0	638	2
80 KUR/LES ¹⁾	EX	298-380	2.52(12)	0	1258±252	2
80 KUR/LES ¹⁾ ¹⁾ k _a + k _b + k _c . Flash-photolysis. Laser Resonance-fluorescence.	EX	298	(3.79±0.60)(10)			2
81 HAC/HOR k _a + k _b + k _c . Discharge-flow. NH ₃ + F → NH ₂ + HF.	EX	248-358	(1.21±0.07)(12)	0	710±48	2
80 BUL/BUL k _b . Flash-photolysis of NH ₃ /O ₃ mixtures. Intra-cavity laser spectroscopy. P(NH ₃) = 5 torr.	EX	298	(7.23±1.81)(10)			2
NH ₂ + H ₂ → NH ₃ + H						
Amidogen + Hydrogen molecule						
80 DEM/LES Flash-photolysis. Resonance-absorption.	EX	300-520	1.26(12)	0	4278±201	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{NH}_2 + \text{NO} \rightarrow [\text{NH}_2\text{NO}] \rightarrow \text{N}_2 + \text{H}_2\text{O}$ (a) $\rightarrow \text{N}_2\text{O} + \text{H}_2$ (b) $\rightarrow \text{N}_2 + \text{H} + \text{OH}$ (c) $\rightarrow \text{N}_2\text{OH} + \text{H}$ (d) $\rightarrow \text{N}_2\text{H} + \text{OH}$ (e)						
Amidogen + Nitrogen oxide (NO)						
72 BED/THO k_a . Reaction of NH_3 with NO_2 in a Pyrex vessel. Photo-multiplier. k_{ref} : $\text{NH}_2 + \text{NO}_2 \rightarrow \text{NH} + \text{HONO}$.	RL	615-660	5.01(-3)	0	-3221±503	2/2
78 SAR/CHE k_a . Pulse photolysis. Laser Spectroscopy.	EX	293	(1.02±0.24)(13)			2
78 ROO/HAN k_a . Shock-waves. NH_2 produced by applying incident shock-waves to a NH_3/NO (or $\text{NH}_3/\text{N}_2\text{O}$) mixture in Ar. Emission and IR-Laser-absorption. The pre-exponential factor expressed as: $A(T/298)^{0.5}$.	ES	1700-3000	8.63(9)	0.5	0	2
79 HAC/SCH2 k_a . Discharge-flow. Resonance-fluorescence. The preexponential factor expressed as: $A(T/298)^{-1.85}$. $P = (0.6-4.0)$ torr.	EX	210-503	7.15(12)	-1.85	0	2
79 NAD/SAR4 k_a . Intracavity laser spectroscopy.	EX	298	1.02(13)			2
81 ROO/HAN ¹⁾ $k_a/(k_a + k_b + k_c + k_d + k_e)$. Estimated ratio.	RL	1680-2850	≈2.3	0	6100	2/2
81 ROO/HAN ¹⁾ k_a . Best data fit.	EX	1680-2850	7.0(13)	0	14000	2 2.0
¹⁾ NH_2 is produced by applying incident shock-waves to a NH_3/NO (or $\text{NH}_3/\text{N}_2\text{O}$) mixture in Ar.						
81 MOR2 $k_a + k_b + k_c + k_d + k_e$. Premixed $\text{H}_2/\text{O}_2/\text{Ar}$ flames. Laser-fluorescence. Upper-limit k . $P = 760$ torr.	EX	1790	<4.82(12)			2
81 ROO/HAN $k_a + k_b + k_c + k_d + k_e$. $M = \text{Ar}$. NH_2 produced by applying incident shock-waves to a NH_3/NO (or $\text{NH}_3/\text{N}_2\text{O}$) mixture in Ar.	EX	1680-2850	3.0(13)	0	7900	2 2.0
81 SCH $k_a + k_b + k_c + k_d + k_e$. Only the initial adduct, and channel (a), detected. Discharge-flow. Resonance-fluorescence. Mass-spectrometry. The preexponential factor expressed as: $A(T/298)^{-1.85}$. $[\text{NO}] = (0.07-1.51) \times 10^{14}$ molec.cm ⁻³ . $P = 1$ torr.	EX	210-503	(7.15±2.12)(12)	-1.85	0	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref)), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 AND/JAC $k_a + k_b + k_c + k_d + k_e$. Isothermal-flow. NH_2 generated by NH_3 Laser-photolysis. Laser-induced Fluorescence. The most important channel is (e).	EX	295	(1.0±0.3)(13)			2
82 SIL/KOL ¹⁾ The preexponential factor expressed as: $A(T/298)^{-2.30}$.	EX	294-1215	(5.38±0.86)(13)	-2.30	684±60	2
82 SIL/KOL ¹⁾ ¹⁾ $k_a + k_b + k_c + k_d + k_e$. Channels (a), (c) and (e) are most important. Reaction of NH_2 with NO in a high-T fast-flow reactor. NH_2 generated by reacting F with NH_3 . $[\text{NO}] = 4.2 \times 10^{13}$ molec.cm ⁻³ . P = (1.0-2.8) torr.	EX	298	5.42(12)			2
82 STI/BRO ²⁾ The preexponential factor expressed as: $A(T/298)^{-1.23}$.	EX	216-480	(1.23±0.40)(13)	-1.23	0	2
82 STI/BRO ²⁾ ²⁾ $k_a + k_b + k_c + k_d + k_e$. Channels (a), (c) and (e) are the most prominent. Flash-photolysis. Laser-induced fluorescence. NH_2 generated by Photolysis of NH_3 in Ar. $P(\text{NH}_3) = (50-250)$ torr. $P(\text{Ar}) = (5-20)$ torr. $P(\text{NO}) < 2.6$ mtorr.	EX	298	(1.26±0.18)(13)			2
$\text{NH}_2 + \text{NO}_2 \rightarrow \text{N}_2\text{O} + \text{H}_2\text{O}$ (a) $\rightarrow \text{N}_2 + \text{H}_2\text{O}_2$ (b) $\rightarrow \text{NH} + \text{HONO}$ (c)						
Amidogen + Nitrogen oxide (NO_2)						
79 HAC/SCH2 $k_a + k_b$. Discharge-flow. Resonance-fluorescence. Channel (a) predominant. Channel (b) probably less than 5%. P = 1 torr. The preexponential factor expressed as: $A(T/298)^{-3.0}$.	EX	250-503	7.18(12)	-3.0	0	2
79 KUR/LES ¹⁾ The preexponential factor expressed as: $A(T/298)^{-1.3}$.	EX	298-505	1.39(13)	-1.3	0	2
79 KUR/LES ¹⁾ ¹⁾ $k_a + k_b$. Flash-photolysis. Resonance-fluorescence. P(Total) = (3.0-10.5) torr.	EX	298	(1.39±0.12)(13)			2
81 SCH $k_a + k_b$. Discharge-flow. Resonance-fluorescence. Mass-spectrometry. P = (1-16) torr. $[\text{NO}_2] = (0.28-8.43) \times 10^{13}$ molec.cm ⁻³ .	EX	250-500	(7.18±1.89)(12)	-3.0	0	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 SCH k _c . Rate constant put on an absolute basis relative to the reaction: NO + NH ₂ → N ₂ + H ₂ O. by using the rate ratio reported in 72 BED/THO. Channel (c) occurs probably at temperatures over 600 K, but not at room temperature.	RN	615-660	1.3(14)	0	2470	2
NH₂ + NH₂ (+ M) → NH₂NH₂ (+ M)						
Amidogen						
71 GOR/MUL Gaseous NH ₃ pulse-radioly	EX	298	6.2(13)			2
73 BAC/YOK	ES	573	(4.7±2.0)(13)			2
77 KHE/SOU ¹⁾ Limiting high-pressure k. No significant T-effect found. P(N ₂) = 1000 torr.	EX	300-500	(1.50±0.75)(13)	0	0	2
77 KHE/SOU ¹⁾ P(N ₂) = 0. (extrapolation to zero-pressure.) E _a = 0 or ±500 cal./mol.	EX	300-500	(8.50±4.25)(14)	0	0	2
79 LOZ/NAD ²⁾ M = Ar, N ₂ . Limiting high-pressure k.	EX	298	(3.61±1.51)(13)			2
79 PAG/ERI Gaseous NH ₃ pulse-radiolysis.	EX	349	1.6(13)			2
71 GEH/HOY M = He. k _{ref} : NH ₂ + NH ₂ → NH + NH ₃	RL	213-473	4.7(6)			3/2
77 KHE/SOU ¹⁾ M = N ₂ . M-efficiencies relative to N ₂ are: 1.0(N ₂), 0.4(Ar), 4.0(NH ₃). No significant T-effect found. At 20 torr. a small negative T-coefficient is observed: -1 < E _a < -0.5 kcal/mol. P < 20 torr.	EX	300-500	(2.55±1.28)(18)	0	0	3
79 LOZ/NAD ²⁾ M = N ₂ . Limiting low-pressure k. M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.42(Ar).	EX	298	(2.50±0.83)(18)			3
¹⁾ Flash-photolysis of NH ₃ .						
²⁾ Intracavity laser spectroscopy.						
Flash-photolysis.						
P = (10-760) torr.						
NH₂ + NH₂NH₂ → NH₃ + NH₂NH						
Amidogen + Hydrazine						
71 GEH/HOY	EX	300	(3.1±0.4)(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units factor	k err.
$\text{NH}_2(^2\text{A}_1) + \text{HN}_3(^1\text{A}') \rightarrow \text{NH}_3(^1\text{A}_1) + \text{N}_3(^2\Pi_g) \text{ (a)}$ $\rightarrow \text{NH}_2(^2\text{B}_1) + \text{HN}_3(^1\text{A}') \text{ (b)}$							
Amidogen + Hydrazoic acid							
80 PIP/KRE k_a . UV photolysis of HN_3 at 290 nm. Laser-induced fluorescence. $P(\text{Tot}) = (5-50)$ torr.	EX	298	5.60(13)				2
78 MCD/MIL $k_a + k_b$. HN_3 photolysis. Gas-chromatography. Channel (b) is predominant.	EX	298	(1.93±0.18)(14)				2
$\text{NH}_2(^2\text{A}_1) + \text{CH}_4 \rightarrow \text{NH}_3(^1\text{A}_1) + \text{CH}_3 \text{ (a)}$ $\rightarrow \text{NH}_2(^2\text{B}_1) + \text{CH}_3 \text{ (b)}$							
Amidogen + Methane							
80 DEM/LES k_a . Flash-photolysis. Resonance-absorption. Tentative k .	ES	300-520	(5.0±2.0)(11)	0	5284±252		2
78 MCD/MIL $k_a + k_b$. HN_3 photolysis. Gas-chromatography. Channel (b) is predominant.	EX	298	(1.81±0.18)(14)				2
$\text{NH}_2 + \text{HCONH}_2 \rightarrow \text{NH}_3 + \text{CONH}_2$							
Amidogen + Formamide							
73 BAC/YOK	ES	573	8.4(9)				2
$\text{NH}_2 + \text{CH}\equiv\text{CH} \rightarrow \text{products (overall)}$							
Amidogen + Ethyne							
81 SCH Discharge-flow. Mass-spectrometry. Same data given in 70 HAC/SCH ₂ . The preeexponential factor expressed as: $A(T/298)^{-2.7}$. $P = (0.4-15)$ torr. $[\text{CH}\equiv\text{CH}] = (0.15-4.16)\times 10^{16}$ molec.cm ⁻³ . $[\text{NH}_2]_0 = (0.05-1.20)\times 10^{13}$ molec.cm ⁻³ .	EX	210-505	(2.92±0.84)(9)	-2.7	0		2
82 BOS NH_3 flash-photolysis. Laser-induced fluorescence. Limiting high-pressure k . $P(\text{Tot}) = (5-100)$ torr.	EX	241-263	(6.69±2.17)(10)	0	1852±100		2
$\text{NH}_2 + \text{CH}_2=\text{CH}_2 \rightarrow \text{products (overall)}$							
Amidogen + Ethene							
79 KHE/LES ¹⁾	EX	300-500	1.2(11)	0	1988±101		2
79 KHE/LES ¹⁾	EX	300	(1.65±0.25)(8)				2
¹⁾ Flash-photolysis. Laser Resonance-absorption. Supersedes 78 LES/KHE.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 SCH Discharge-flow. Mass-spectrometry. Same data given in 79 HAC/SCH2. $[\text{CH}_2=\text{CH}_2] = (0.04-3.07) \times 10^{16} \text{ molec.cm}^{-3}$. $[\text{NH}_2]_0 = (0.08-1.59) \times 10^{13} \text{ molec.cm}^{-3}$. P = (0.4-10.5) torr.	EX	295-505	(1.3±0.7)(9)	0	0	2
82 BOS Ammonia Flash-photolysis. Laser-induced fluorescence. P(Tot) = (5-100) torr.	EX	250-365	(2.05±0.07)(10)	0	1318±23	2
$\text{NH}_2(^2\text{A}_1) + \text{CH}_2=\text{CH}_2 \rightarrow \text{NH}_3(^1\text{A}_1) + \text{CH}_2=\text{CH} \quad (\text{a})$ $\rightarrow \text{NH}_2(^2\text{B}_1) + \text{CH}_2=\text{CH}_2 \quad (\text{b})$						
Amidogen + Ethene						
78 MCD/MIL $k_a + k_b$. HN_3 photolysis. Channel (b) predominant.	EX	298	(1.87±0.18)(14)			2
$\text{NH}_2 + \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{NH}_2 \quad (\text{a})$ $\rightarrow \text{NH}_3 + \text{CH}_2=\text{CH}_2 \quad (\text{b})$						
Amidogen + Ethyl						
82 DEM/LES $k_a + k_b$. Flash-photolysis. Resonance-Absorption. NH_2 and CH_3CH_2 generated by flashing NH_3 in presence of $\text{CH}_2=\text{CH}_2$. Best-fit by simulation. Supersedes 78 LES/DEM.	DE	298	(2.5±0.5)(13)			2
$\text{NH}_2 + \text{CH}_3\text{CH}_3 \rightarrow \text{NH}_3 + \text{CH}_3\text{CH}_2$						
Amidogen + Ethane						
80 DEM/LES Flash-photolysis. Resonance-absorption.	EX	300-520	3.7(11)	0	3598±141	2
$\text{NH}_2 + \text{CH}_2=\text{C}=\text{CH}_2 \rightarrow \text{products (overall)}$						
Amidogen + 1,2-Propadiene						
81 SCH Discharge-flow. Mass-spectrometry. Upper-limit k. $[\text{CH}_2=\text{C}=\text{CH}_2] = (0.4-1.39) \times 10^{16} \text{ molec.cm}^{-3}$. P = 1 torr. Same data given in 79 HAC/SCH2.	EX	298	≤5.0(8)			2
$\text{NH}_2 + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{products (overall)}$						
Amidogen + 1-Propene						
76 LES/SOU	EX	300-500	2.9(11)	0	2164±101	2
76 LES/SOU	EX	300	(2.2±0.3)(8)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 KHE/LES ¹⁾	EX	300-500	2.8(11)	0	2164±101	2
79 KHE/LES ¹⁾	EX	300	(2.15±0.35)(8)			2
¹⁾ Flash-photolysis. Resonance-absorption. Supersedes 78 LES/KHE.						
81 SCH	EX	298	≤6.0(8)			2
Discharge-flow. Resonance-fluorescence. Mass-spectrometry. Upper-limit k. [CH ₃ CH=CH ₂] = (2.10-2.77)×10 ¹⁶ molec.cm ⁻³ . P = 1 torr. Same data given in 79 HAC/SCH2.						
NH ₂ + $\triangle$ → products (overall)						
Amidogen + Cyclopropane						
81 SCH	EX	250-300	(1.9±0.6)(8)	0	0	2
Discharge-flow. Mass-spectrometry. [Cyclopropane] = (0.49-7.83)×10 ¹⁶ molec.cm ⁻³ . [NH ₂] ₀ = (0.36-2.41)×10 ¹³ molec.cm ⁻³ . P = (7.5-15) torr.						
NH ₂ (² A ₁) + $\triangle$ → NH ₃ + $\triangle^{\bullet}$ (a)						
→ NH ₂ (¹ B ₁) + $\triangle$ (b)						
Amidogen + Cyclopropane						
78 MCD/MIL	EX	298	(1.87±0.18)(14)			2
k _a + k _b . HN ₃ photolysis. Channel (b) predominant.						
NH ₂ + (CH ₃) ₂ CH → (CH ₃) ₂ CHNH ₂ (a) → NH ₃ + CH ₃ CH=CH ₂ (b)						
Amidogen + Ethyl, 1-methyl-						
82 DEM/LES	DE	298	(2.0±0.4)(13)			2
k _a + k _b . Flash-photolysis. Resonance-absorption. NH ₂ and (CH ₃) ₂ CH generated by flashing NH ₃ in presence of 1-Propene. Best-fit by simulation. Supersedes 78 LES/DEM.						
NH ₂ + CH ₃ CH ₂ CH ₃ → NH ₃ + CH ₃ CH ₂ CH ₂ (a) → NH ₃ + (CH ₃) ₂ CH (b)						
Amidogen + Propane						
80 DEM/LES	EX	300-520	4.5(11)	0	3095±126	2
k _a + k _b . Flash-photolysis. Resonance-absorption.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
NH₂ + CH₂=CHCH=CH₂ → products						
Amidogen + 1,3-Butadiene						
81 SCH ¹⁾	EX	230-360	(3.8±1.3)(11)	0	1140	2
81 SCH ¹⁾	EX	298	(6.7±2.3)(9)			2
¹⁾ Discharge-flow. Mass-spectrometry. [CH ₂ =CHCH=CH ₂] = (0.03-1.20)×10 ¹⁶ molec.cm ⁻³ . [NH ₂] ₀ = (0.22-1.33)×10 ¹³ molec.cm ⁻³ .						
82 HAC/SCH	EX	230-360	3.8(11)	0	1140	2
Discharge-flow. NH ₃ + F → NH ₂ + HF. [1,3-Butadiene] ₀ < 1.0×10 ¹⁶ molec.cm ⁻³ . [NH ₂] ₀ = (0.2-1.2)×10 ¹³ mole.cm ⁻³ . P = (1.5-7.5)						
NH₂ + CH₃CH₂CH=CH₂ → products						
Amidogen + 1-Butene						
79 KHE/LES ¹⁾	EX	300-500	2.8(11)	0	2063±101	2
79 KHE/LES ¹⁾	EX	300	(3.00±0.45)(8)			2
¹⁾ Flash-photolysis. Resonance-absorption.						
NH₂ + cis-CH₃CH=CHCH₃ → products						
Amidogen + 2-Butene, (Z)-						
79 KHE/LES ¹⁾	EX	300-500	3.3(11)	0	2164±101	2
79 KHE/LES ¹⁾	EX	300	(2.55±0.40)(8)			2
¹⁾ Flash-photolysis. Resonance-absorption.						
NH₂ + trans-CH₃CH=CHCH₃ → products						
Amidogen + 2-Butene, (E)-						
79 KHE/LES ¹⁾	EX	300-500	3.5(11)	0	2139±101	2
79 KHE/LES ¹⁾	EX	300	(2.95±0.45)(8)			2
¹⁾ Flash-photolysis. Resonance-absorption.						
NH₂ + (CH₃)C=CH₂ → products						
Amidogen + 1-Propene, 2-methyl-						
79 KHE/LES ¹⁾	EX	300-500	4.6(11)	0	2265±101	2
79 KHE/LES ¹⁾	EX	300	(2.55±0.40)(8)			2
¹⁾ Flash-photolysis. Resonance-absorption.						
NH₂ + (CH₃)₃C → (CH₃)₃CNH₂ (a) → NH₃ + (CH₃)₂C=CH₂ (b)						
Amidogen + Ethyl, 1,1-dimethyl-						
82 DEM/LES	ES	298	(2.5±0.5)(13)			2
k _a + k _b . Flash-photolysis. Resonance-absorption. Best-fit by simulation. Supersedes 78 LES/DEM.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{NH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{NH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$ (a) $\rightarrow \text{NH}_3 + \text{CH}_3\text{CH}_2\text{CHCH}_3$ (b)						
Amidogen + Butane						
80 DEM/LES $k_a + k_b$. Flash-photolysis. Resonance-absorption.	EX	300-520	7.0(11)	0	3070±126	2
$\text{NH}_2 + (\text{CH}_3)_3\text{CH} \rightarrow \text{NH}_3 + (\text{CH}_3)_3\text{C}$ (a) $\rightarrow \text{NH}_3 + (\text{CH}_3)_2\text{CHCH}_2$ (b)						
Amidogen + Propane, 2-methyl-						
79 KHE/LES ¹⁾	EX	300-500	2.4(11)	0	2516±101	2
79 KHE/LES ¹⁾	EX	300	(6.2±0.9)(7)			2
¹⁾ Flash-photolysis. Resonance-absorption.						
80 DEM/LES $k_a + k_b$. Flash-photolysis. Resonance-absorption.	EX	300-520	2.3(11)	0	2466±111	2
$\text{NH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{NH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ (a) $\rightarrow \text{NH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3$ (b) $\rightarrow \text{NH}_3 + (\text{CH}_3\text{CH}_2)_2\text{CH}$ (c)						
Amidogen + Pentane						
80 HAC/HOR $k_a + k_b + k_c$. Discharge-flow. $\text{NH}_3 + \text{F} \rightarrow \text{NH}_2 + \text{HF}$.	EX	250-360	3.7(10)	0	1227	2
$\text{NH}_3 (+\text{M}) \rightarrow \text{NH}_2 + \text{H} (+\text{M})$ (a) $\rightarrow \text{NH} + \text{H}_2 (+\text{M})$ (b)						
Ammonia						
73 GEN/ZHI k_a . M = Ar. Limiting high-pressure k.	EX	2200-2600	6.61(12)	0	49321±2516	1 3.47
72 HAL k_a . M = Ar.	EX	1989-2693	1.0(14)	0	42386	2
73 GEN/ZHI k_a . M = Ar. Limiting low-pressure k.	EX	2300-3100	5.76(15)	0	38752±2516	2 6.31
77 FIS k_a . M = H ₂ O. Rich NH ₃ /O ₂ /N ₂ flames.	ES	1950-2100	2.7(16)	0	42406	2
80 ROO/HAN ¹⁾	DE	2200-3450	2.52(16)	0	47200	2
80 ROO/HAN ¹⁾	DE	2798	1.19(9)			2
¹⁾ k_a . M = Ar. NH ₃ decomposition behind incident shock-waves. Data-fit. P = (0.14-0.6) atm.						
80 YUM/ASA ²⁾ [NH ₃] ₀ = (0.03-4.8)×10 ¹⁵ molec.cm ⁻³ . [Ar] = (0.3-5.4)×10 ¹⁸ molec.cm ⁻³ .	EX	2050-3070	1.38(16)	0	45596	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k(k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
81 YUM/ASA ²⁾ [NH ₃] ₀ = (0.6-4.8)x10 ¹⁴ molec.cm ⁻³ . [Ar] = (0.02-1.2)x10 ¹⁹ molec.cm ⁻³ . ²⁾ k _a . M = Ar. Thermolysis of NH ₃ behind incident shock-waves. Vacuum-UV Absorption-spectroscopy.	EX	1740-3050	1.78(16)	0	46351±1711	2	2.14
80 ROO/HAN ³⁾ k _b .	DE	2798	3.4(6)			2	
80 ROO/HAN ³⁾ k _b /k _a .	RL	2798	≤1.0(-2)			2/2	
³⁾ NH ₃ decomposition behind incident shock-waves. Rate constant and rate ratio determined by computer simulation. P = (0.14-0.6) atm.							
73 VOM1 k _a + k _b . M = Ne.	EX	2300-3200	2.51(14)	0	33216±2013	2	2.0
72 HAL k _a + k _b . M = Ar. Overall decomposition.	EX	1989-2693	4.12(12)	0	41983	2	
79 DOV/NIP k _a + k _b . Pyrolysis behind reflected shock-waves. M = (88.9-99.7)% Kr + (0.16-5.0)% Ar. Data-fit.	EX	2500-3000	1.2(16)	0	45798	2	2.0
81 HOL/WAG ⁴⁾ k _a + k _b . M = Ar. Limiting low-pressure k.	EX	200-330	4.0(16)	0	47272	2	
81 HOL/WAG ⁴⁾ k _a + k _b . M = Ar. Extrapolated limiting high-pressure k.	EX	2200-3300	5.5(15)	0	54250	1	
⁴⁾ Thermolysis of NH ₃ behind shock-waves. Total density = 5.4x10 ¹⁷ -1.2x10 ²⁰ molec.cm ⁻³ .							
NH₃ + HONO → products							
Ammonia + Nitrous acid							
78 KAI/JAP2 Discharge-flow. Upper-limit k.	EX	300	≤9.03(6)			2	
NH₃ + CH₂=CHCN → NH₂CH₂CH₂CN							
Ammonia + 2-Propenenitrile (Acrylonitrile) → Propanenitrile, 3-amino- (β-Aminopropionitrile)							
82 SAI/MIC Reaction in an Autoclave.	EX	303-408	6.55(13)	0	9109	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
NH=NH → products						
Diazenes						
73 WIL/BAC Decomposition in gas phase at 295 K. The only products observed: N ₂ , H ₂ , and NH ₂ NH ₂ . Ammonia not observed, but cannot be ruled out.	EX	295	(3.8±0.5)(-3)			1
cis-NH=NH + CH₂=CHCH=CH₂ → N₂ + CH₃CH₂CH=CH₂ Diazenes, (Z)- + 1,3-Butadiene						
74 VID/WIL k _{ref} : cis-NH=NH + CH ₂ =CH ₂ → N ₂ + CH ₃ CH ₃ Estimated ratio.	RL	373	(6.5±0.7)(-2)			2/2
cis-NH=NH + cis-CH₃CH=CHCH₃ → N₂ + CH₃CH₂CH₂CH₃ Diazenes, (Z)- + 2-Butene, (Z)-						
74 VID/WIL k _{ref} : cis-NH=NH + CH ₂ =CH ₂ → N ₂ + CH ₃ CH ₃ Estimated ratio.	RL	373	(1.1±0.1)(-1)			2/2
cis-NH=NH + trans-CH₃CH=CHCH₃ → N₂ + CH₃CH₂CH₂CH₃ Diazenes, (Z)- + 2-Butene, (E)-						
74 VID/WIL k _{ref} : cis-NH=NH + CH ₂ =CH ₂ → N ₂ + CH ₃ CH ₃ Estimated ratio.	RL	373	(3.3±0.3)(-1)			2/2
cis-NH=NH +  → N₂ +  Diazenes, (Z)- + 1,3-Cyclohexadiene						
74 VID/WIL k _{ref} : cis-NH=NH + CH ₂ =CH ₂ → N ₂ + CH ₃ CH ₃ Estimated ratio.	RL	373	(5.0±0.2)(-2)			2/2
cis-NH=NH + (CH₃)₂C=C(CH₃)₂ → N₂ + (CH₃)₂CHCH(CH₃)₂ Diazenes, (Z)- + 2-Butene, 2,3-dimethyl-						
74 VID/WIL k _{ref} : cis-NH=NH + CH ₂ =CH ₂ → N ₂ + CH ₃ CH ₃ Estimated ratio.	RL	373	(2.0±0.1)(-2)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	E, B-B(ref)	k, A units	k err. factor
$\text{trans-NH=NH} \rightarrow \text{cis-NH=NH}$ (a)							
$\text{trans-NH=NH} + \text{cis-NH=NH} \rightarrow \text{NH}_2\text{NH}_2 + \text{N}_2$ (b)							
$\rightarrow \text{trans-NH=NH} + \text{N}_2 + \text{H}_2$ (c)							
Diazene, (E)-							
77 WIL/BAC $k_a + k_b + k_c$.	EX	296-433	3.0	0	2114	1	
74 VID/WIL k_a .	ES	373	$\sim 1.0(-2)$			1	
77 WIL/BAC k_a . Determined from the above mechanism.	ES	296-433	1.8	0	2114	1	
74 VID/WIL k_b/k_{ref} . Estimated ratio.	RL	373	(6.0 ± 2.0)			2/2	
k_{ref} : $\text{cis-NH=NH} + \text{CH}_2=\text{CH}_2 \rightarrow \text{N}_2 + \text{CH}_3\text{CH}_3$							
77 WIL/BAC k_b/k_c . Determined from the above mechanism.	RL	296-433	2.33			2/2	
$\text{trans-ND=ND} \rightarrow \text{cis-ND=ND}$ (a)							
$\text{trans-ND=ND} + \text{cis-ND=ND} \rightarrow \text{ND}_2\text{ND}_2 + \text{N}_2$ (b)							
$\rightarrow \text{trans-ND=ND} + \text{N}_2 + \text{D}_2$ (c)							
Diazene-d ₂ , (E)-							
77 WIL/BAC $k_a + k_b + k_c$.	EX	296-433	2.0	0	2214	1	
77 WIL/BAC k_a . Determined from the above mechanism.	ES	296-433	1.0	0	2214	1	
77 WIL/BAC k_b/k_c . Determined from the above mechanism.	RL	296-433	4.9(1)			2/2	
$\text{NH}_2\text{NH} + \text{NH}_2\text{NH} \rightarrow \text{NH}_3 + \text{NH}_3 + \text{N}_2$							
Hydrazyl							
79 PAG/ERI Gaseous NH_3 pulse-radiolysis.	EX	349	1.0(14)			2	
$\text{NH}_2\text{NH}_2 (+\text{M}) \rightarrow \text{NH}_2 + \text{NH}_2 (+\text{M})$							
Hydrazine							
74 GEN/ZHI M = Ar. Limiting high-pressure k.	EX	1100-1400	3.98(13)	0	26673 $\pm$ 1007	1	2.51
$\text{HN}_3 (+\text{M}) \rightarrow \text{NH}(^1\Delta) + \text{N}_2(^1\Sigma_g^+) (+\text{M})$ (a)							
$\rightarrow \text{NH}(^3\Sigma^-) + \text{N}_2(^1\Sigma_g^+) (+\text{M})$ (b)							
Hydrazoic acid							
72 ZAS/KOG $k_a + k_b$. M = Ar. Channel (a) is predominant.	EX	1045-1450	1.78(11)	0	20131	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k _A k err. units factor
79 KAJ/YAM k _a + k _b . M = Ar. HN ₃ Thermolysis. Channel (b) is predominant in this T-range. P(Ar) = (600-2200) torr.	EX	1200-1350	7.59(14)	0	18218±805	2 1.9
82 DUP/PAI ¹⁾	EX	1250-1400	5.5(13)	0	14000	2
82 DUP/PAI ¹⁾	EX	1450-2000	2.2(12)	0	9750	2
¹⁾ k _a + k _b . M = Ar. Thermolysis of HN ₃ in Ar behind incident shock-waves. 0.5% HN ₃ . (98-99.5)% Ar. Channel (a) is predominant.						
79 KAJ/YAM k _b . NH ₃ pyrolysis. P(Ar) = (600-2200) torr.	EX	1200-1350	7.59(13)	0	15702±1007	2 2.24
HNO + HNO → H₂O + N₂O (a)						
→ H₂O₂ + N₂ (b)						
Nitrosyl hydride						
73 WIE/HEI k _a /k _b . T-independent k.	RL	298-423	5.1(1)	0	0	2/2
75 CAL/CAR k _a . Flash Photolysis of H ₂ /NO mixtures. HNO absorption at 207.3 nm.	EX	295	(3.22±1.08)(9)			2
81 CHE/NAD k _a . CH ₃ CHO/HCHO/NO flash-photolysis. Intracavity Laser-spectroscopy. P(NO) = (6-20) torr. P(HCHO) = 7 torr. P(CH ₃ CHO) = 12.2 torr.	EX	298	(9.03±4.82)(8)			2
DNO + DNO → D₂O + N₂O						
Nitrosyl hydride-d						
75 CAL/CAR D ₂ /NO flash-photolysis. 206.4 nm. DNO absorption.	EX	295	(1.31±0.48)(9)			2
HONO (+ M) → OH + NO (+ M)						
Nitrous acid						
76 FIF M = Ar. Limiting high-pressure k.	EX	1000-1400	≥5.5(12)	0	24157	1
HONO† → OH + NO						
Nitrous acid						
76 OVE/PAR M = H ₂ O, CF ₂ , SF ₆ , N ₂ , Ar, or He. HONO† formed by OH + NO.	EX	295	(1.18±0.186)(9)			1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
HONO + O₃ → HONO₂ + O₂							
Nitrous acid + Ozone							
77 KAI/JAP ¹⁾	EX	226	≤3.01(5)				2
77 KAI/JAP ¹⁾	EX	300	≤6.02(4)				2
¹⁾ Upper limit k's.							
P(Tot) = (20-30) torr.							
79 STR/WEL	EX	296	≤(2.71±1.81)(5)				2
Upper-limit k.							
HONO + HONO → NO + HO₂ + H₂O							
Nitrous acid							
75 ENG/COR	RN	298	5.6(6)				2
75 ENG/COR	DE	298-323	(1.10±0.21)(13)	0	4320±62		2
A and B recalculated from the reported data.							
Optimization. k ₁ = k ₋₁ K.							
76 CHA/NOR	EX	296	(5.71±1.63)(5)				2
HONO + HONO₂ → NO₂ + NO₂ + H₂O							
Nitrous acid + Nitric acid							
74 ENG/COR	EX	298	(5.85±0.31)(6)				2
74 ENG/COR	EX	298-323	(3.71±0.48)(12)	0	3987±41		2
A and B recalculated from the reported data.							
77 KAI/WU	EX	300	(9.34±1.81)(6)				2
79 STR/WEL	EX	296	6.63(6)				2
HONO₂ (+ M) → OH + NO₂ (+ M)							
Nitric acid							
74 GLA/TRO1 ¹⁾	EX	900-1200	≈2.0	0	24660		1
Extrapolated limiting high-pressure k.							
74 GLA/TRO1 ¹⁾	RN	295-1200	1.26(15)	0	24006		1 1.58
Limiting high-pressure k over extended T-range.							
73 GER/DEM	EX	1013-1170	1.39(15)	0	16105±906		2 2.00
M = He.							
74 GLA/TRO1 ¹⁾	EX	900-1200	≈2.2(17)	0	20130		2
Extrapolated, Limiting low-pressure k.							
Concentration-dependent Arrhenius							
expression = k/[Ar].							
74 GLA/TRO1 ¹⁾	RN	295-1200	1.10(20)	-1.98	24006		2 1.58
Extended T-range, limiting low-pressure k.							
Concentration-dependent Arrhenius							
expression = k/[Ar]. The preexponential							
factor expressed as: A(T/298) ^{-1.98} .							
¹⁾ M = Ar.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 BAS/KOG	EX	863-1173	6.0(14)	0	15148±1596	2	4.68
79 GER/DEM	EX	1050-1200	1.69(15)	0	16105±906	2	2.0
M = He.							
M-efficiencies relative to He are:							
1.0(He), 0.77(Ar), 1.1(N ₂). P = (2-5) torr.							
 HO ₂ NO ₂ (+ M) → HO ₂ + NO ₂ (+ M) (a) → HONO + O ₂ (+ M) (b)							
Peroxynitric acid							
77 GRA/WIN ¹⁾	EX	254-283	1.4(14)	0	10418±252	1	1.1
77 COX/DER ¹⁾	EX	300-328	1.26(16)	0	11700±110	1	39.8
78 GRA/WIN ¹⁾	EX	278	~1.8(-2)			1	
M = N ₂ . Limiting high-pressure k.							
77 SIM/HEI ¹⁾	RN	245-328	6.0(17)	0	13085	1	
78 SIM/HEI ¹⁾ ²⁾	RN	245-328	6.31(17)	0	13085±2516	1	
Δlogk = 3.5.							
¹⁾ k _a .							
78 SIM/HEI ²⁾	RL	245-328	3.0(9)	0	5788	1/1	
k _a /k _b .							
78 SIM/HEI ²⁾	EX	245-328	1.0(8)	0	7046±755	1	10.0
k _b .							
²⁾ N ₂ O/H ₂ /O ₂ /NO photolysis.							
78 GRA/WIN	EX	261-295	3.13(18)	0	10015±252	2	
k _a . M = N ₂ .							
M-efficiencies relative to N ₂ are:							
1.00(N ₂), 0.83(O ₂). Limiting low-pressure k.							
 NH ₂ O → NHOH							
Nitroxide							
80 BUL/BUL	EX	298	(1.3±0.1)(3)			1	
 NH ₂ O + O ₃ → NH ₂ + O ₂ + O ₂							
Nitroxide + Ozone							
80 BUL/BUL	EX	298	(1.2±0.9)(10)			2	
 NH ₂ O ₂ [†] → NH ₂ + O ₂ (a) → HNO + OH (b)							
Aminodioxo							
81 FUJ/MIY1 ¹⁾	DE	300-2200	(1.0±0.3)(10)	0	0	1	
k _a .							
81 FUJ/MIY1 ¹⁾	DE	300-2200	(1.3±0.3)(10)	0	0	1	
k _b .							
¹⁾ Oxidation of NH ₃ behind reflected shock-waves.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
C + O₂ → CO + O						
Carbon atom + Oxygen molecule						
71 HUS/KIR3 Vacuum-UV Time-Resolved Resonance Radiation.	EX	300	(1.99±0.90)(13)			2
75 HUS/YOU	EX	300	(1.57±0.18)(13)			2
C(2¹D₂) (+ M) → products						
Carbon atom						
71 HUS/KIR2 M = CO. M-efficiencies relative to CO are: 1.00(CO), 2.31(CO ₂), 2.94(NO), 8.75(N ₂ O), 8.75(N ₂ O), 13.13(CH ₄), ~1.63(O ₂), ~1.06(H ₂ O), ~23.13(CH ₂ =CH ₂).	EX	300	(9.64±3.61)(12)			2
C(2¹D₂) + H₂ → CH + H						
Carbon atom + Hydrogen molecule						
71 HUS/KIR1	EX	300	(1.57±0.18)(14)			2
C + H₂ (+ M) → CH₂ (+ M)						
Carbon atom + Hydrogen molecule						
71 HUS/KIR3 M = He. Vacuum-UV Time-Resolved Resonance Radiation.	EX	300	(2.58±0.91)(16)			3
75 HUS/YOU M = He.	EX	300	(2.5±0.44)(16)			3
C + H₂O → CO + N₂ (a) → HCHO (b)						
Carbon atom + Water						
71 HUS/KIR3 k _a + k _b . Vacuum-UV Time-Resolved Resonance Radiation. Upper-limit k.	EX	300	≤2.17(11)			2
75 HUS/YOU k _a + k _b . Upper-limit k.	EX	300	<6.02(11)			2
C + N₂ (+ M) → CN₂ (+ M)						
Carbon atom + Nitrogen molecule						
71 HUS/KIR3 M = Ar. Vacuum-UV Time-Resolved Resonance Radiation.	EX	300	(1.12±0.54)(15)			3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
C + NO → CN + O						
Carbon atom + Nitrogen oxide (NO)						
71 HUS/KIR3 Time-Resolved Resonance Radiation.	EX	300	(4.40±1.33)(13)			2
75 HUS/YOU	EX	300	(2.89±0.49)(13)			2
C + N₂O → CO + N₂ (a) → CN + NO (b)						
Carbon atom + Nitrogen oxide (N ₂ O)						
71 HUS/KIR3 k _a + k _b . Time-Resolved Resonance Radiation.	EX	300	(1.51±0.96)(13)			2
75 HUS/YOU k _a + k _b .	EX	300	(7.83±1.81)(12)			2
C + C (+ M) → C₂ (+ M)						
Carbon atom						
76 SLA M = Ar. Based on reverse reaction measurements. The preexponential factor expressed as: A(T/298) ^{-1.6} .	ES	5000-6000	(1.98±1.10)(17)	-1.6	0	3
C + CO (+ M) → C₂O (+ M)						
Carbon atom + Carbon monoxide						
71 HUS/KIR3 M = He. Vacuum UV Time-Resolved Resonance Radiation.	EX	300	(2.29±0.98)(16)			3
C + CO₂ → CO + CO						
Carbon atom + Carbon dioxide						
71 HUS/KIR3 Time-Resolved Resonance-Radiation. Upper-limit k.	EX	300	<6.02(9)			2
75 HUS/YOU Upper-limit k.	EX	300	<6.02(8)			2
C + CH₂ → H₂ + C₂(d³Π_g)						
Carbon atom + Methylene						
82 GRE/HOM2 Reaction of the CH=CH/CH/O/H system, diluted in N ₂ /He carrier gas. Discharge-flow. Resonance-fluorescence. O atoms generated by reacting N with NO. P = 2 torr.	EX	298	≈7.0(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
C + CH₄ → CH₂=CH₂						
Carbon atom + Methane						
71 HUS/KIR3 Time-Resolved Resonance-Radiation. Upper-limit k.	EX	300	<1.20(9)			2
C + CN → C₂ + N						
Carbon atom + Cyanogen						
76 SLA	ES	5000-8000	(3.0±1.5)(14)	0	18118	2
C + O=C=C=O → products						
Carbon atom + 1,2-Propadiene-1,3-dione						
75 HUS/YOU	EX	300	(1.08±0.12)(14)			2
C(¹S₀) + O=C=C=O → products						
Carbon atom + 1,2-Propadiene-1,3-dione						
74 HUS/KIR	EX	300	6.02(13)			2
CO + O₂ → CO₂ + O						
Carbon monoxide + Oxygen molecule						
71 BRA/BEL1	ES	1300-1900	1.6(13)	0	20634	2 3.47
71 DEA/KIS Shock-waves. Best-fit to experimental data.	DE	1750-2575	1.20(13)	0	30196	2
74 RAW/GAR1 Shock-waves.	EX	1500-2500	1.2(11)	0	17614	2
76 WEI	EX	2500-2900	2.5(13)	0	24157	2
CO + O₃ → products						
Carbon monoxide + Ozone						
72 ARI/WAR Upper-limit k. Possible products: CO ₂ + O ₂ .	EX	296	≤2.41(-1)			3
73 STE/NIK2 Upper-limit k.	EX	298	≤6.02(2)			2
CO + SO₂(³B₁) → CO₂ + SO						
Carbon monoxide + Sulfur dioxide						
77 SU/CAL Photolysis of SO ₂ /CO mixtures.	EX	298	2.60(9)			2
CO + NO₂ → CO₂ + NO						
Carbon monoxide + Nitrogen oxide (NO ₂)						
76 MIL	EX	950-1500	3.24(13)	0	16105±654	2 1.78
77 FRE/PAL	EX	1309-1946	2.19(13)	0	14696±805	2 1.66

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 FRE/PAL Best fit. Preferred k.	SE	298-2000	8.9(13)	0	17011	2	2.0
79 MIL/ADA Single-pulse shock-tube.	EX	950-1500	3.24(13)	0	16105±654	2	1.78
80 PAL/FRE Incident shock-waves. P = (10-70) torr.	EX	950-1950	8.91(13)	0	17011	2	
 $\text{CO} + \text{NO}_2(^2\text{B}_2) \rightarrow \text{CO}_2 + \text{NO}$ Carbon monoxide + Nitrogen oxide (NO_2)e							
76 HER/MAR At (506±1) nm.	EX	298	7.23(8)			2	
76 HER/MAR At 750 nm.	EX	298	1.33(8)			2	
78 HER/MAR Laser-induced fluorescence. At 488 nm.	EX	298	(1.93±0.72)(9)			2	
 $\text{CO} + \text{N}_2\text{O} \rightarrow \text{CO}_2 + \text{N}_2$ Carbon monoxide + Nitrogen oxide (N_2O)							
73 MIL/MAT	EX	1169-1655	2.09(11)	0	8707±1158	2	2.29
76 MIL	EX	1169-1655	7.08(11)	0	10569±1057	2	2.19
79 ZAS/LOS ¹⁾ In 76% Ar.	EX	1700-2500	2.75(15)	0	25164±604	2	5.75
79 ZAS/LOS ¹⁾ In 97% Ar.	EX	1500-1900	7.08(14)	0	26673±2013	2	2.0
¹⁾ Exchange reaction behind reflected shock-waves.							
 $\text{CO}_2 (+\text{M}) \rightarrow \text{CO} + \text{O} (+\text{M})$ Carbon dioxide							
74 WAG/ZAB M = Ar. Limiting high-pressure k.	EX	2740-3700	9.0(12)	0	65274	1	
73 DEA M = Ar.	EX	3700-5600	6.31(13)	0	42637±926	2	1.23
74 HAR/VAS M = Ar. In Aluminum shock-tubes. Low P.	EX	3400-4400	2.7(14)	0	53347	2	
74 HAR/VAS M = Ar. In Brass shock-tubes. Low P.	EX	2700-4300	4.7(14)	0	52843	2	
74 KIE M = Kr. Shock waves.	EX	3600-6503	3.89(14)	0	53951±503	2	
74 WAG/ZAB M = Ar. Concentration-dependent Arrhenius expression = k[Ar]. Limiting low-pressure k.	EX	3000-4561	5.1(14)	0	55561	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 EBR/SAN The preexponential factor expressed as: $A(T/298)^{0.5}$.	EX	2500-7000	1.29(14)	0.5	52340±1258	2
CO₂ + C₂O → products						
Carbon dioxide + Carbon oxide (C ₂ O)						
80 DON/PIT Laser photodissociation of C ₃ O ₂ at 266 nm. Dye-laser induced fluorescence. Upper-limit k.	EX	298	<6.02(9)			2
CH + O₂ → CO + OH(A²Σ⁺) (a)						
→ CO ₂ + H (b)						
→ CHO + O (c)						
→ CO + O + H (d)						
Methylidyne + Oxygen molecule						
79 MES/SAD k _a . Laser-induced fluorescence.	EX	298	(1.99±0.24)(13)			2
82 GRE/HOM1 Ethyne/O/H reaction in He/N ₂ . Discharge-flow. Resonance-fluorescence. Best-fit. O atoms generated reacting N with NO. H atoms produced by a discharge of a H ₂ /He mixture. P = 2 torr.	EX	298	4.8(10)			2
71 BOS/PER k _a + k _b + k _c + k _c . Upper-limit k.	EX	298	≤2.4(13)			2
81 BUT/FLE k _a + k _b + k _c + k _d . Multiphoton dissociation of CHBr ₃ at 193 nm. Laser-induced fluorescence. Same data in 80 BUT/FLE. P(Total) = 100 torr.	EX	298	(3.55±0.48)(13)			2
82 BER/FLE2 k _a + k _b + k _c + k _d . M = Ar. Laser-photolysis/LIF. CH generated by CHBr ₃ Multiphoton dissociation at 266 nm. and monitored by LiF at 430 nm.	EX	297-676	(3.25±0.60)(13)	0	0	2
CH + H₂ → products						
Methylidyne + Hydrogen molecule						
71 BOS/PER	EX	298	(1.05±0.12)(13)			2
79 BUT/GOS Multiphoton photodissociation of CHBr ₃ . Laser-Induced Multiphoton Fluorescence. P ~ 2mtorr.	EX	298	(1.39±0.30)(13)			2
81 BUT/FLE Multiphoton dissociation of CHBr ₃ at 193 nm. Laser-Induced Fluorescence. Same data in 80 BUT/FLE. P(Total) = 100 torr.	EX	298	(1.57±0.30)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH + H₂O → products						
Methylidyne + Water						
71 BOS/PER	EX	298	(2.7±0.5)(13)			2
CH + N₂ (+ M) → CHN₂ (+ M) (a)						
→ [HCN ₂] → HCN + N (+ M) (b)						
Methylidyne + Nitrogen molecule						
71 BOS/PER	EX	298	(6.1±1.0)(11)			2
k _a .						
79 BUT/GOS	EX	298	(4.64±1.20)(11)			2
k _a . CHBr ₃ Multiphoton dissociation.						
Laser-induced Fluorescence. P = 2 torr.						
81 BUT/FLE	EX	298	(5.60±0.60)(11)			2
k _a . CHBr ₃ Multiphoton dissociation at 193 nm.						
Laser-induced fluorescence.						
P(CHBr ₃) = (5-50) mtorr.						
P(Total) = 100 torr.						
Same data given in 80 BUT/FLE.						
82 WAG/CAR ¹)	ES	298	(3.79±0.78)(11)			2
k _b . Limiting high-pressure k.						
82 WAG/CAR ¹)	ES	298	(9.43±0.11)(16)			3
k _b . Limiting low-pressure k.						
¹) Laser-induced fluorescence.						
CH generated by Multiphoton dissociation						
of CH ₃ CN, or CH ₃ NH ₂ in Ar.						
CH + NO → CO + NH (a)						
→ CN + OH (b)						
→ HCN + O (c)						
→ HCO + N (d)						
→ CNO + H (e)						
Methylidyne + Nitrogen oxide (NO)						
82 LE	ES	2700	6.0(14)			2
k _a . Premixed fuel-rich Ethyne/NO flames,						
at 250-600 nm.						
P = 80 torr.						
81 BUT/FLE	EX	298	(1.75±0.42)(14)			2
k _a + k _b + k _c + k _d + k _e .						
CHBr ₃ Multiphoton dissociation at 193 nm.						
Laser-induced-fluorescence.						
P(CHBr ₃) = (5-50) mtorr.						
P(Total) = 100 torr.						
Same data given in 80 BUT/FLE.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 BER/FLE2 $k_a + k_b + k_c + k_d + k_e$. M = Ar. Laser-photolysis/LIF. CH generated by CHBr_3 Multiphoton dissociation at 266 nm. P(Total) 100 torr. (Ar).	EX	297-676	(1.14±0.18)(14)	0	0	2
82 WAG/CAR $k_a + k_b + k_c + k_d + k_e$. Laser-induced Fluorescence. CH generated by IR-Multiphoton dissociation of CH_3NH_2 , or Cyclopropane in Ar. P(Ar) = 5 torr.	EX	298	(1.20±0.18)(13)			2
CH + $\text{NO}_2 \rightarrow \text{NH} + \text{CO}_2$ (a) $\rightarrow \text{CO} + \text{HNO}$ (b) $\rightarrow \text{CHO} + \text{NO}$ (c) $\rightarrow \text{HCN} + \text{O}_2$ (d) $\rightarrow \text{CO} + \text{NO} + \text{H}$ (e) $\rightarrow \text{NCO} + \text{OH}$ (f)						
Methylidyne + Nitrogen oxide (NO_2)						
82 WAG/CAR $k_a + k_b + k_c + k_d + k_e + k_f$. Laser-induced Fluorescence. CH generated by IR-Multiphoton dissociation of CH_3CN , or CH_3NH_2 , or Cyclopropane in Ar. P(Ar) = 5 torr.	EX	298	(1.00±0.06)(13)			2
CH + $\text{N}_2\text{O} \rightarrow \text{products}$						
Methylidyne + Nitrogen oxide N_2O						
82 WAG/CAR Laser-induced fluorescence. CH generated by IR-Multiphoton dissociation of CH_3NH_2 , or Cyclopropane in Ar. P(Ar) = 20 torr.	EX	298	(4.70±0.84)(13)			2
CH + $\text{NH}_3 \rightarrow \text{products}$						
Methylidyne + Ammonia						
71 BOS/PER	EX	298	5.9(10)			2 1.17
CH + CO $\rightarrow \text{products}$						
Methylidyne + Carbon monoxide						
71 BOS/PER	EX	298	2.9(12)			2
81 BUT/FLE 193 nm. CHBr_3 Multiphoton dissociation at 193 nm. at 193 nm. Laser induced fluorescence. Same data given in 80 BUT/FLE. P(CHBr_3) = (5-50) mtorr. P(Total) = 100 torr.	EX	298	(1.26±0.18)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 BER/FLE2 Reaction of CH with CO in Ar. Laser-photolysis/ LIF. CH generated by CHBr ₃ Multiphoton dissociation at 266 nm. P(Total) = 100 torr.(Ar)	EX	297-676	(2.77±0.60)(11)	0	-861±101	2	
CH + CO₂ → products							
Methylidyne + Carbon dioxide							
81 BUT/FLE CHBr ₃ Multiphoton dissociation at 193 nm. Laser-induced fluorescence. Same data given in 80 BUT/FLE. P(Total) 100 torr. P(CHBr ₃) = (5-50) mtorr.	EX	298	(1.14±0.24)(12)			2	
82 BER/FLE2 M = Ar. Laser-photolysis/LIF. CH generated by CHBr ₃ Multiphoton dissociation at 266 nm. P(Total) = 100 torr.(Ar)	EX	297-676	(3.43±0.54)(12)	0	345±53	2	
CH + CH₂ → H₂ + CH=C*							
Methylidyne + Methylene							
82 GRE/HOM2 Reaction of the CH=CH/O/H in N ₂ /He. Discharge-flow. Resonance-fluorescence. Lower-limit k. P = 2 torr.	EX	298	≥1.0(14)			2	
CH + CH₄ → products							
Methylidyne + Methane							
71 BOS/PER	EX	298	(2.01±0.05)(13)			2	
79 BUT/GOS CHBr ₃ Multiphoton photodissociation. Laser-induced fluorescence. Superseded by 81 BUT/FLE. P ~ 2 mtorr.	EX	298	(1.81±0.60)(14)			2	
81 BUT/FLE CHBr ₃ Multiphoton dissociation at 193 nm. Laser-induced fluorescence. P(CHBr ₃) = (5-50) mtorr. P(Total) = 100 torr. Same data given in 80 BUT/FLE.	EX	298	(6.02±1.81)(13)			2	
CH + CH=CH → products							
Methylidyne + Ethyne							
71 BOS/PER	EX	298	4.5(13)			2	1.2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 FLE/FUJ CHBr ₃ Multiphoton dissociation at 193 nm. Laser-induced fluorescence.	EX	298	(8.42±2.71)(13)			2
81 BUT/FLE CHBr ₃ Multiphoton dissociation at 193 nm. Laser-induced fluorescence. P(CHBr ₃) = (5-50) mtorr. P(Total) = 100 torr.	EX	298	(1.33±0.24)(14)			2
82 BER/FLE1 M = Ar. Laser-photolysis/LIF. CH generated by CHBr ₃ Multiphoton dissociation at 266 nm. Before forming the products, CH adds to the triple bond, giving the intermediate:  P(Total) = 100 torr. (Ar)	EX	160-652	(2.10±0.25)(14)	0	-61±36	2
CH + CH ₂ =CH ₂ →  → CH ₂ =CHCH ₂ (a)						
→ any other products (b)						
Methylidyne + Ethene						
82 BER/FLE1 k _a . M = Ar. Laser-photolysis/LIF. CH generated by CHBr ₃ Multiphoton dissociation at 266 nm. P(Total) = 100 torr. (Ar)	EX	171-657	(1.34±0.16)(14)	0	-173±35	2
71 BOS/PER k _{overall} .	EX	298	(6.9±0.6)(13)			2
80 FLE/FUJ k _{overall} . CHBr ₃ Multiphoton dissociation at 193 nm. Laser-induced fluorescence.	EX	298	(1.54±0.08)(14)			2
81 BUT/FLE k _{overall} . CHBr ₃ Multiphoton dissociation at 193 nm. Laser-induced fluorescence. P(CHBr ₃) = (5-50) mtorr. P(Total) = 100 torr.	EX	298	(1.26±0.48)(14)			2
CH + CH ₃ CH ₃ → products						
Methylidyne + Ethane						
81 BUT/FLE CHBr ₃ Multiphoton dissociation at 193 nm. Laser induced fluorescence. Same data given in 80 BUT/FLE. P(Total) = 100 torr. P(CHBr ₃) = (5-50) mtorr.	EX	298	(2.41±0.6)(14)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH + CH₃C≡CH → products							
Methylidyne + 1-Propyne							
80 FLE/FUJ Multiphoton dissociation of CHBr ₃ at 193 nm. Laser-induced fluorescence.	EX	298	(2.64±0.51)(14)			2	
81 BUT/FLE Multiphoton dissociation of CHBr ₃ at 193 nm. Laser-induced fluorescence. P(Total) = 100 torr.	EX	298	(2.77±0.90)(14)			2	
CH +  → products							
Methylidyne + Cyclopropane							
81 BUT/FLE Multiphoton dissociation of CHBr ₃ at 193 nm. Laser-induced fluorescence. P(Total) = 100 torr.	EX	298	(1.44±0.42)(14)			2	
CH + CH₃CH₂CH₃ → products							
Methylidyne + Propane							
71 BOS/PER	EX	298	8.2(13)			2	1.2
CH + CH₃CH₂CH₂CH₃ → products							
Methylidyne + Butane							
71 BOS/PER	EX	298	(7.8±0.7)(13)			2	
81 BUT/FLE Multiphoton dissociation of CHBr ₃ at 193 nm. Laser-induced fluorescence. P(Total) = 100 torr. Same data given in 80 BUT/FLE.	EX	298	(3.49±0.30)(14)			2	
CH +  → products							
Methylidyne + Cyclohexane							
81 BUT/FLE Multiphoton dissociation of CHBr ₃ at 193 nm. Laser-induced fluorescence. P(Total) = 100 torr.	EX	298	(2.77±1.14)(14)			2	
CH₂(X³B₁) + O₂ → products							
Methylene + Oxygen molecule							
73 JON/BAY2 k _{ref} : CH ₂ + O → CO + H + H.	RL	296	(9.5±3.0)(-2)			2/2	
73 PEE/MAH2	ES	1200-1600	1.0(14)	0	1860	2	
74 LAU/BAS M = He. Limiting high-pressure k.	EX	298	(9.03±0.60)(11)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 PEE/VIN1	ES	2000	$\approx 1.2(13)$			2	
75 PEE/VIN2	RL	1500-2200	≈ 3.0			2/2	
$k_{\text{ref}}: \text{OH} + \text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_2$. Average ratio.							
75 PEE/VIN2	RN	1500-2200	$\approx 1.2(13)$	0	0	2	
NH_4/O_2 and $\text{CH}_2=\text{CH}_2/\text{O}_2$ flames, diluted in Ar. k determined relative to reaction: $\text{OH} + \text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_2$							
77 PIL/ROB	ES	298	7.23(11)			2	
79 VIN/DEB1 ¹⁾	EX	295-600	1.33(13)	0	755 $\pm$ 151	2	1.55
79 VIN/DEB2 ¹⁾	EX	295	(1.02 $\pm$ 0.24)(12)			2	
¹⁾ $\text{CH}\equiv\text{CH}$ oxidation. Fast-flow. P(Total) 2.2 torr.							
$\text{CH}_2(a^1A_1) + \text{O}_2 \rightarrow \text{products}$ Methylene + Oxygen molecule							
74 LAU/BAS	EX	298	$< 1.81(13)$			2	
M = He. Limiting high-pressure, upper-limit k.							
$\text{CH}_2(X^3B_1) + \text{H}_2 \rightarrow \text{CH}_3 + \text{H}$ Methylene + Hydrogen molecule							
77 PIL/ROB	ES	298	$< 3.01(9)$			2	
Upper-limit k.							
$\text{CH}_2(a^1B_1) + \text{H}_2 \rightarrow \text{CH}_3 + \text{H}$ Methylene + Hydrogen molecule							
77 PIL/ROB	ES	298	1.20(13)			2	
$\text{CH}_2(^1A_1) + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{OH}$ Methylene + Water							
81 HAT/BAN	RN	298	$\approx 1.81(12)$			2	
Diazomethane Photolysis in air, or N_2 , in presence of Water. P(Diazomethane) $\sim$ 9 mtorr. P(air, or N_2) = 760 torr. P(H_2O) = (0-4) torr. k estimated relative to the reaction: $\text{CH}_2(^1A_1) + \text{CH}_2\text{N}\equiv\text{N} \rightarrow \text{CH}_2=\text{CH}_2 + \text{N}_2$							
$\text{CH}_2(X^3B_1) + \text{N}_2 \rightarrow \text{HCN} + \text{NH}$ Methylene + Nitrogen molecule							
78 LAU/BAS	EX	300	$\leq 6.02(7)$			2	
Flash-photolysis of $\text{CH}_2\text{CO}/\text{N}_2$ and $\text{CH}_2\text{N}_2/\text{N}_2$ systems. Upper-limit k.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₂(X³B₁) + NO → CH₂NO → products						
Methylene + Nitrogen oxide (NO)						
74 LAU/BAS M = He. Limiting high-pressure k.	EX	298	(9.64±0.60)(12)			2
77 PIL/ROB	ES	298	6.02(12)			2
79 VIN/DEB1 CH≡CH oxidation. Fast-flow. P(Total) = 2.2 torr.	EX	295-600	(1.39±0.83)(12)	0	-554±201	2
CH₂(a¹A₁) + NO → products						
Methylene + Nitrogen oxide (NO)						
74 LAU/BAS M = He. Limiting high-pressure, upper-limit k.	EX	298	<2.41(13)			2
CH₂(X³B₁) + CO → CH≡CH + O (a) → any other products (b)						
Methylene + Carbon monoxide						
81 TSU/HAS k _a . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ mixtures behind reflected shock-waves.	ES	1200-1800	1.34(13)	0	26943	2
74 LAU/BAS k _{overall} . Limiting high-pressure, upper-limit k.	EX	298	6.02(8)			2
CH₂(a¹A₁) + CO → products						
Methylene + Carbon monoxide						
74 LAU/BAS M = He. Limiting high-pressure, upper-limit k.	EX	298	<5.42(12)			2
CH₂(X³B₁) + CO₂ → HCHO + O₂						
Methylene + Carbon dioxide						
77 LAU/BAS	EX	298	2.3(10)			2 1.5
CH₂(X³B₁) + CH₃ → CH₂=CH₂ + H						
Methylene + Methyl						
75 LAU/BAS1	EX	295	6.0(13)			2 1.3
75 PIL/ROB Computer fit.	DE	298	3.0(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
78 OLS/GAR Shock-waves. Absorption-spectroscopy. Best data-fit to a proposed mechanism. Total conc.: $\sim 7.2 \times 10^{17}$ molec.cm ⁻³ .	DE	1800-2700	2.00(13)	0	0	2
$\text{CH}_2(\text{X}^3\text{B}_1) + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_3$						
Methylene + Methane						
73 HAL/CRU ¹⁾ $k_{\text{ref}}: \text{CH}_2(\text{X}^3\text{B}_1) + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3(\text{CH}_2)_3\text{CH}_3$	RL	304	(4.3±0.2)(-1)			2/2
73 HAL/CRU ¹⁾ $k_{\text{ref}}:$ $\text{CH}_2(\text{X}^3\text{B}_1) + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3(\text{CH}_2)_3\text{CH}_3$ (a) $\rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3$ (b)	RL	304	(2.3±0.1)(-1)			2/2
¹⁾ Limiting high-pressure k.						
$\text{CH}_2(\text{X}^3\text{B}_1) + \text{CH}_2=\text{N}=\text{N} \rightarrow \text{CH}_2=\text{CH}_2 + \text{N}_2$						
Methylene + Methane, diazo-						
71 BEL Diazomethane/Propane Photolysis. Gas-Chromatography. Estimated ratio. $k_{\text{ref}}: \text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2$ (a) $\rightarrow \text{CH}_3 + (\text{CH}_3)_2\text{CH}$ (b)	RL	298	(4.0±1.0)(2)			2/2
$\text{CH}_2(\text{a}^1\text{A}_1) + \text{CH}_2=\text{N}=\text{N} \rightarrow \text{CH}_2=\text{CH}_2 + \text{N}_2$						
Methylene + Methane, diazo-						
71 BEL Diazomethane/Propane Photolysis. Gas-Chromatography.	ES	298	(1.87±0.60)(13)			2
81 HAT/BAN Diazomethane photolysis in air or N ₂ , in presence of H ₂ O. $k_{\text{ref}}: \text{CH}_2(\text{a}^1\text{A}_1) + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{OH}$. P(Diazomethane) ~ 9 mtorr. P(air, or N ₂) = 760 torr. P(H ₂ O) = (0-4) torr.	RL	298	(1.8±0.6)(1)			2/2
$\text{CH}_2(\text{X}^3\text{B}_1) + \text{CH}=\text{CH} \rightarrow \text{CH}_2=\text{C}=\text{CH}_2$ (a) $\rightarrow \text{CH}_3\text{C}\equiv\text{CH}$ (b)						
Methylene + Ethyne						
74 LAU/BAS $k_a + k_b$. Limiting high-pressure k.	EX	298	(4.52±0.60)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
77 PIL/ROB $k_a + k_b$.	ES	298	2.41(12)			2
79 VIN/DEB2 $k_a + k_b$. CH=CH oxidation. Fast-flow. The intermediate step: $\text{CH}_2(\text{X}^3\text{B}_1) + \text{CH}=\text{CH} \rightarrow \text{CH}_2\text{C}=\text{CH} + \text{H}$ is suggested, leading to the products of channels (a) and (b). P(Total) = 2.2 torr.	EX	295	(7.83±1.81)(11)			2
 $\text{CH}_2(\text{X}^3\text{B}_1) + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3$ Methylene + Ethane						
73 HAL/CRU ¹⁾ $k_{\text{ref}}: \text{CH}_2(\text{X}^3\text{B}_1) + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_3$	RL	304	2.52			2/2
73 HAL/CRU ¹⁾	RN	304	2.89(12)			2
73 HAL/CRU ¹⁾ $k_{\text{ref}}: \text{CH}_2(\text{X}^3\text{B}_1) + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3(\text{CH}_2)_3\text{CH}_3$	RL	304	(1.08±0.01)			2/2
73 HAL/CRU ¹⁾ $k_{\text{ref}}:$ $\text{CH}_2(\text{X}^3\text{B}_1) + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3(\text{CH}_2)_3\text{CH}_3$ (a) $\rightarrow (\text{CH}_3)_2\text{CHCHH}_2\text{CH}_3$ (b)	RL	304	(5.8±0.1)(-1)			2/2
73 HAL/CRU ¹⁾ $k_{\text{ref}}:$ $\text{CH}_2(\text{X}^3\text{B}_1) + (\text{CH}_3)_3\text{CH} \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3$	RL	304	(7.4±0.4)(-1)			2/2
73 HAL/CRU ¹⁾ $k_{\text{ref}}:$ $\text{CH}_2(\text{X}^3\text{B}_1) + (\text{CH}_3)_3\text{CH} \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3$ (a) $\rightarrow (\text{CH}_3)_4\text{C}$ (b)	RL	304	(6.5±0.3)(-1)			2/2
¹⁾ Insertion at primary CH bond.						
 $\text{CH}_2(\text{a}^1\text{A}_1) + \text{CH}_2=\text{C}=\text{O} \rightarrow \text{CH}_2=\text{CH}_2 + \text{CO}$ Methylene + Ethenone (Ketene)						
74 LAU/BAS M = He. Limiting high-pressure k.	EX	298	(1.93±0.72)(13)			2
77 PIL/ROB	ES	298	2.11(12)			2
 $\text{CH}_2(\text{a}^1\text{B}_1) + \text{CH}_2=\text{C}=\text{O} \rightarrow \text{CH}_2=\text{CH}_2 + \text{CO}$ Methylene + Ethenone (Ketene)						
77 PIL/ROB	ES	298	1.81(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CD}_2 + \text{CD}_2=\text{C}=\text{O} \rightarrow \text{CD}_2=\text{CD}_2 + \text{CO}$						
Methylene-d ₂ + Ethenone-d ₂ (Ketene-d ₂)						
71 MCN/KEL	RL	653	6.6			2/2
$k_{\text{ref}}:$						
$\text{CD}_2 + (\text{CH}_3)_4\text{C} \rightarrow \text{CD}_2\text{H} + (\text{CH}_3)_3\text{CCH}_2$						
$\text{CH}_2(\text{X}^3\text{B}_1) + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ (a)						
$\rightarrow (\text{CH}_3)_3\text{CH}$ (b)						
Methylene + Propane						
73 HAL/CRU	RL	304	3.32			2/2
$(k_a + k_b)/k_{\text{ref}}.$						
$k_{\text{ref}}:$						
$\text{CH}_2(\text{X}^3\text{B}_1) + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_3$						
73 HAL/CRU	RL	304	$(8.0 \pm 0.2)(-1)$			2/2
$(k_a + k_b)/k_{\text{ref}}.$						
$k_{\text{ref}}:$						
$\text{CH}_2(\text{X}^3\text{B}_1) + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3(\text{CH}_2)_3\text{CH}_3$ (a)						
$\rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3$ (b)						
73 HAL/CRU	RN	304	3.79(12)			2
$k_a + k_b.$						
73 HAL/CRU ¹⁾	ES	304	2.65(12)			2
$k_a.$ Insertion at primary CH bond.						
73 HAL/CRU ¹⁾	ES	304	1.14(12)			2
$k_b.$ Insertion at secondary CH bond.						
¹⁾ Recalculated from the reported 1.20 efficiency of CH ₂ insertion at secondary over primary bonds in Propane.						
73 HAL/CRU	RL	304	1.02			2/2
$k_a/k_{\text{ref}}.$						
Insertion at primary CH bond.						
$k_{\text{ref}}:$						
$\text{CH}_2(\text{X}^3\text{B}_1) + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3(\text{CH}_2)_3\text{CH}_3$						
73 HAL/CRU	RL	304	$(4.4 \pm 0.11)(-1)$			2/2
$k_b/k_{\text{ref}}.$						
Insertion at secondary CH bond.						
$k_{\text{ref}}:$						
$\text{C}_2(\text{X}^3\text{B}_1) + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3(\text{CH}_2)_3\text{CH}_3$						
73 HAL/CRU	RL	304	$(2.4 \pm 0.11)(-1)$			2/2
$k_b/k_{\text{ref}}.$						
Insertion at secondary CH bond.						
$k_{\text{ref}}:$						
$\text{C}_2(\text{X}^3\text{B}_1) + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3(\text{CH}_2)_3\text{CH}_3$ (a)						
$\rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3$ (b)						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2(a^1A_1) + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \text{ (a)}$ $\rightarrow (\text{CH}_3)_3\text{CH} \text{ (b)}$						
Methylene + Propane						
71 BEL ¹⁾ k_a .	ES	298	(2.65±0.72)(12)			2
71 BEL ¹⁾ k_b .	ES	298	(1.14±0.30)(12)			2
71 BEL ¹⁾ $k_a + k_b$.	ES	298	(3.79±1.02)(12)			2
¹⁾ Dizomethane-Propane Photolysis. Gas-chromatography.						
75 ZAB/CAR $k_a + k_b$. k_{ref} :	RL	298	1.67(1)			2/2
$\text{CH}_2(a^1A_1) + \text{M} \rightarrow \text{CH}_2(X^3B_1) + \text{M}$.						
$\text{CH}_2(a^1A_1) + \text{CH}_2=\text{CHCH}=\text{CH}_2 \rightarrow \text{cis-CH}_2\text{CH}=\text{CHCH}=\text{CHCH}_3 \text{ (a)}$ $\rightarrow \text{trans-CH}_2=\text{CHCH}=\text{CHCH}_3 \text{ (b)}$ $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}=\text{CH}_2 \text{ (c)}$ $\rightarrow \triangle \text{CH}=\text{CH}_2 \text{ (d)}$						
Methylene + 1,3-Butadiene						
75 CRA/ROS $(k_a + k_b + k_c)/k_d$. Bond insertion versus bond addition.	RL	298	1.4(-1)			2/2
$\text{CH}_2(X^3B_1) + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \text{ (a)}$ $\rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \text{ (b)}$						
Methylene + Butane						
73 HAL/CRU $(k_a + k_b)/k_{\text{ref}}$. k_{ref} :	RL	304	4.28			2/2
$\text{CH}_2(X^3B_1) + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_3$						
73 HAL/CRU $k_a + k_b$.	RN	304	4.88(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
73 HAL/CRU ¹⁾ k _a . Insertion at primary CH bond.	ES	304	2.59(12)			2	
73 HAL/CRU ¹⁾ k _b . Insertion at secondary CH bond.	ES	304	2.29(12)			2	
¹⁾ Recalculated from the reported 1.31 efficiency of CH ₂ insertion at secondary over primary CH bonds in Butane.							
73 HAL/CRU k _b /k _a . Secondary versus primary CH insertion.	RL	304	(8.8±0.1)(-1)			2/2	
CH ₂ (a ¹ A ₁) + CH ₃ CH ₂ CH ₂ CH ₃ → CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ [†] (a) → (CH ₃) ₂ CHCH ₂ CH ₃ [†] (b)							
Methylene + Butane							
72 GRO/HAS ¹⁾ (k _a + k _b)/k _{ref} .	RL	298	1.89			2/2	
72 GRO/HAS ¹⁾ k _b /k _{ref} .	RL	298	(8.9±0.07)(-1)			2/2	
¹⁾ k _{ref} : CH ₂ (a ¹ A ₁) + CH ₃ CH ₃ → CH ₃ CH ₂ CH ₃ [†]							
CH ₂ (X ³ B ₁) + (CH ₃) ₃ CH → (CH ₃) ₂ CHCH ₂ CH ₃ (a) → (CH ₃) ₄ C (b)							
Methylene + Propane, 2-methyl-							
73 HAL/CRU (k _a + k _b)/k _{ref} . k _{ref} : CH ₂ (X ³ B ₁) + CH ₄ → CH ₃ CH ₃	RL	304	3.89			2/2	
73 HAL/CRU k _a + k _b .	RN	304	4.46(12)			2	
73 HAL/CRU ¹⁾ k _a . Insertion at primary CH bond.	ES	304	3.88(12)			2	
73 HAL/CRU ¹⁾ k _b . Insertion at tertiary CH bond.	ES	304	5.80(12)			2	
¹⁾ Recalculated from the reported 1.33 efficiency of CH ₂ insertion at secondary over primary CH bonds in 2-Methylpropane.							
73 HAL/CRU k _b /k _a . Tertiary versus primary CH insertion.	RL	304	(1.5±0.1)(-1)			2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2(a^1A_1) + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (a)						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$ (b)						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ (c)						
Methylene + Pentane						
75 ZAB/CAR	RL	298	1.11(1)			2/2
$k_a + k_b + k_c$.						
$k_{\text{ref}}: \text{CH}_2(a^1A_1) + \text{M} \rightarrow \text{CH}(X^3B_1) + \text{M}$.						
$\text{CD}_2 + (\text{CH}_3)_4\text{C} \rightarrow \text{CD}_2\text{H} + (\text{CH}_3)_3\text{CCH}_2$						
Methylene- d_2 + Propane, 2,2-dimethyl-						
71 MCN/KEL	RL	653	(2.1±0.5)			2/2
$k_{\text{ref}}: \text{CD}_2 + \text{CD}_2=\text{C}=\text{O} \rightarrow \text{CD}_3 + \text{CD}=\text{C}=\text{O}$						
71 MCN/KEL	RN	653	1.5(11)			2 1.5
$\text{CH}_3 (+ \text{M}) \rightarrow \text{CH}_2 + \text{H} (+ \text{M})$						
Methyl						
80 BHA/FRA	EX	1700-2300	6.1(15)	0	44900	2
M = Ar. Shock-tube. Atomic Resonance-Absorption.						
80 ROT/BAR	EX	2150-2850	1.95(16)	0	46100	2
M = Ar. Ethane Thermolysis behind shock-waves.						
Atomic Resonance-Absorption. Same data in 79 ROT/BAR and 80 ROT. Total conc. $\sim 4.0 \times 10^{18}$ molec. cm^{-3} .						
$\text{CH}_3 + \text{O}_2 (+ \text{M}) \rightarrow \text{HCHO} + \text{O} + \text{H} (+ \text{M})$ (a)						
$\rightarrow \text{CH}_3\text{O} + \text{O} (+ \text{M})$ (b)						
$\rightarrow \text{CO} + \text{OH} + \text{H}_2 (+ \text{M})$ (c)						
$\rightarrow \text{HCHO} + \text{OH} (+ \text{M})$ (d)						
$\rightarrow \text{CH}_3\text{O}_2 (+ \text{M})$ (e)						
Methyl + Oxygen molecule						
80 BHA/FRA	EX	1700-2300	7.0(12)	0	12910	2
k_a . Shock-tube. Absorption-spectrometry.						
75 BRA/BRO	EX	1200-1800	2.4(13)	0	14500	2
k_b .						
78 REI/ROM	CO	300-2000	1.69(13)	0	15350	2
k_b . RRKM calculation.						
72 SKI/LIF	ES	1000-2500	4.0(12)	0	9059	2
k_c .						
75 BOW1	ES	1900-2400	1.2(11)	0	5000	2
k_d . Best data-fit.						
76 TSU	DE	1500-2000	9.0(11)	0	6014	2
k_d . Computer calculation.						
76 WAS/BAY	EX	259-341	1.74(11)	0	940±250	2 2.24
k_d .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
71 CLA/IZO2 k _d . Shock-waves and TOF Mass-spectrometry. Total conc. = 9×10^{13} molec.cm ⁻³ .	ES	1350	1.99(10)			2
71 DEA/KIS k _d . Shock-waves. Best data-fit. Total conc. = 5×10^{17} molec.cm ⁻³ .	DE	1750-2575	3.01(13)	0	5033	2
71 IZO/KIS k _d . Shock waves. Best data-fit. Total conc. = 5×10^{17} molec.cm ⁻³ .	DE	1400-2200	1.20(12)	0	6291	2
78 OLS/GAR k _d . Shock-waves. Absorption-spectroscopy. Best data-fit. Total conc. = $\sim 7.2 \times 10^{17}$ molec.cm ⁻³ .	DE	1800-2700	6.92(11)	0	4530	2
78 REI/ROM k _d . RRKM Calculation.	CO	300-2000	1.69(11)	0	4982	2
79 KLA/AND k _d . Flash-photolysis. Resonance-fluorescence. Upper-limit k.	EX	368	$\leq 1.81(8)$			2
79 TAB/BAU k _d . M = Ar. CH ₄ oxidation in shock-waves. Best data-fit on the basis of a proposed mechanism. Total conc. = $(2.3-4.4) \times 10^{18}$ molec.cm ⁻³ .	ES	1950-2770	2.70(12)	0	6039	2
80 BHA/FRA k _d . Shock-tube. Atomic Resonance-Absorption Spectrometry. Upper-limit k.	EX	1700-2300	$\leq 5.2(13)$	0	17400	2
80 BOR/ZAM k _d . Spontaneous ignition of CH ₄ /O ₂ /N ₂ O mixtures.	EX	880-1670	2.00(12)	0	6714	2
80 WAS k _d . M = He. Generation of CH ₃ by reaction of O with CH ₂ =CH ₂ . Fast-flow reactor. Photoionization Mass-spectrometry. k measurements by both, Stern-Volmer plots and steady-state. Comparable data given in 79 WAS1, 79 WAS2, and 79 WAS3. P(CH ₂ =CH ₂) ₀ = (0.30-0.65) mtorr. P(O) ₀ = (0.04-0.19) mtorr. P(Total) = (1.9-6.0) torr. P(O ₂) = (48-229) mtorr.	EX	298	$(1.02 \pm 0.96)(10)$			2
81 BOR/DRA k _d . Combustion of CH ₄ /O ₂ mixtures behind reflected shock-waves. P = 750 torr.	EX	880-1670	2.00(12)	0	6670	2
82 PAR k _d . Reaction of CH ₄ with O ₂ in single-pulse shock-waves. Mass-spectrometry.	EX	1097	3.96(10)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 PLU/RVA2 k _d . Reaction of CH ₃ with O ₂ in a flow-reactor, in He. CH ₃ generated by reacting F with CH ₄ . F atoms generated by dissociation of CF ₄ in a microwave-discharge. Mass-spectrometry. Upper-limit k. [CH ₃] ₀ = (3.7-9.3)x10 ¹⁰ molec.cm ⁻³ . [CF ₄] ₀ = (2.5-7.5)x10 ¹¹ molec.cm ⁻³ . [He] = (0.2-2.1)x10 ¹⁷ molec.cm ⁻³ . [CH ₄] = (8-12)x10 ¹² molec.cm ⁻³ . [O ₂] = 5.2x10 ¹⁵ molec.cm ⁻³ .	EX	295	≤1.81(8)			2
71 VAN/CAL k _e . M = CH ₃ CH ₂ CH ₃ . Limiting high pressure k.	ES	295	~1.1(12)			2
72 BAS/JAM k _e . M = N ₂ , or (CH ₃) ₄ C. Limiting high-pressure k.	EX	295	(3.1±0.3)(11)			2
73 SOK/NIK k _e . M = He. Limiting high-pressure k.	EX	453	1.5(12)			2
75 LAU/BAS2 k _e . M = He, Ar, N ₂ . Limiting high-pressure k.	RN	298	1.02(12)			2
77 HOC/GHO k _e . M = H ₂ . Limiting high-pressure k.	EX	295	(1.3±0.2)(12)			2
77 PAR k _e . M = N ₂ . Limiting high-pressure k.	EX	298	(7.23±3.61)(11)			2
72 BAS/JAM k _e . M = (CH ₃) ₄ C. Low-pressure k.	EX	295	(3.6±0.3)(17)			3
72 BAS/JAM k _e . M = N ₂ . Low-pressure k.	EX	295	(9.4±0.3)(16)			3
73 SOK/NIK k _e . M = He. Low-pressure k.	EX	453	3.9(16)			3
77 PAR k _e . M = N ₂ . Low-pressure k.	EX	298	(1.12±0.79)(17)			3
77 PAR k _e . M = (CH ₃) ₄ C. Low-pressure k.	EX	298	(5.44±2.90)(17)			3
80 WAS k _e . M = He. Generation of CH ₃ by reaction of O with CH ₂ =CH ₂ Fast-flow reactor. Photoionization Mass-spectrometer. k measurements by both, Stern-Volmer plots and steady-state. Comparable data given in 79 WAS1, 79 WAS2 and 79 WAS3. P(Total) = (1.9-6.0) torr. P(CH ₂ =CH ₂) ₀ = (0.30-0.65) mtorr. P(O) ₀ = (0.04-0.19) mtorr. P(O ₂) = (48-339) torr.	EX	298	(5.80±4.35)(16)			3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 FLU/RYA2 k _e . Flow-reactor. CH ₃ generated by reacting F with CH ₄ in He. F atoms generated by dissociation of CF ₄ in a Microwave-discharge. Limiting low-pressure k. [CH ₃] ₀ = (3.7-9.3)x10 ¹⁰ molec.cm ⁻³ . [CF ₄] ₀ = (2.5-7.5)x10 ¹¹ molec.cm ⁻³ . [He] = (0.2-2.1)x10 ¹⁷ molec.cm ⁻³ . [CH ₄] = (8-12)x10 ¹² molec.cm ⁻³ . [O ₂] = 5.2x10 ¹⁵ molec.cm ⁻³ .	EX	295	(1.23±0.40)(17)			3
CD ₃ + O ₂ → DCDO + OD Methyl-d ₃ + Oxygen molecule						
80 CHI/SKI CD ₄ oxidation in CD ₄ /O ₂ /Ar behind reflected shock-waves. Resonance-absorption spectroscopy.	EX	1700-2200	6.8(11)	0	4571	2
CH ₃ + O ₃ → CH ₃ O + O ₂ (a) → HCHO + H + O ₂ (b)						
Methyl + Ozone						
75 SIM/HEI ¹⁾	RL	221	1.2			2/2
75 SIM/HEI ¹⁾	RL	298	2.2			2/2
¹⁾ (k _a + k _b)/k _{ref} . k _{ref} : CH ₃ + O ₂ → CH ₃ O ₂						
75 SIM/HEI k _a + k _b .	RN	221-298	3.25(12)	0	528	2
80 WAS/AKI M = He. Generation of CH ₃ by reaction of O with CH ₂ =CH ₂ . Fast-flow. Photoionization Mass-Spectrometry. k measurements by Stern-Volmer plots. 3 other possible channels suggested. Comparable data reported in 79 WAS1, 79 WAS2 and 79 WAS3. P(O) ₀ = (0.16-0.40) mtorr. P(CH ₂ =CH ₂) ₀ = (0.36-0.45) mtorr. P(Total) = (1.9-5.7) torr.	EX	298	(4.22±1.63)(11)			2
81 OGR/PAL ²⁾ n = 0 assumed.	EX	243-384	(3.25±0.90)(12)	0	216±80	2
81 OGR/PAL ²⁾ The preexponential factor expressed as: A(T/298) ^{0.71} .	EX	243-384	(1.56±0.42)(12)	0.71	0	2
²⁾ k _a + k _b . M = He. Flash-photolysis of CH ₃ O ₂ at 193 nm. with an ArF laser, in a O ₃ /O ₂ /He mixture. P(Total) = (2-4) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃ + H₂ → CH₄ + H							
Methyl + Hydrogen molecule							
72 SHA/WES k _{ref} : CH ₃ + D ₂ → CH ₃ D + D.	RL	398-718	(9.11±0.20)(-1)	0	-668±12	2/2	
73 CLA/DOV2	EX	1340	(4.6±1.4)(10)			2	
73 CLA/DOV2	ES	1200-2000	1.55(13)	0	7801	2	2.0
74 KOB/PAC The preexponential factor expressed as: A(T/298) ^{2.0} .	EX	372-1370	7.05(10)	2.0	4811	2	
81 MAR/SHA Azomethane Decomposition in H ₂ . Flow-system. P(Total) = (5-26) torr.	EX	584-671	5.01(11)	0	5293	2	
CH₃[*] + H₂ → CH₄ + H							
Methyl + Hydrogen molecule							
73 TIN/WES k _{ref} : CH ₃ [*] + CH ₃ Br → CH ₄ + CH ₂ Br. CH ₃ [*] is a 'hot' radical formed by photolysis of CH ₃ Br at 185 nm.	RL	298	(7.5±0.25)(-2)			2/2	
CH₃ + HD → CH₄ + D							
Methyl + Deuterium hydride							
72 SHA/WES k _{ref} : CH ₃ + DH → CH ₃ D + H	RL	398-718	(2.83±2.58)(-1)	0	-971±347	2/2	
CH₃ + D₂ → CH₃D + D							
Methyl + Deuterium molecule							
76 PRA/ROG2	EX	300-1118	1.60(12)	0	6369±41	2	1.08
77 YAN k _{ref} : CH ₃ + CH ₃ CH=CH ₂ → CH ₄ + CH ₂ CH=CH ₂ Estimated ratio.	RL	1260-1390	3.4(-1)			2/2	
CH₃[*] + D₂ → CH₃D + D							
Methyl + Deuterium molecule							
73 TIN/WES k _{ref} : CH ₃ [*] + CH ₃ Br → CH ₄ + CH ₂ Br. CH ₃ [*] is a 'hot' radical formed by photolysis of CH ₃ Br at 185 nm.	RL	298	(8.00±0.13)(-2)			2/2	
CD₃ + H₂ → CD₃H + H							
Methyl-d ₃ + Hydrogen molecule							
72 SHA/WES k _{ref} : CD ₃ + D ₂ → CD ₄ + D.	RL	398-718	(1.592±0.124)	0	-296±35	2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CD}_3^* + \text{H}_2 \rightarrow \text{CD}_3\text{H} + \text{H}$ Methyl-d ₃ + Hydrogen molecule 73 TIN/WES $k_{\text{ref}}: \text{CD}_3^* + \text{CD}_3\text{Br} \rightarrow \text{CD}_4 + \text{CD}_2\text{Br}.$ CD_3^* is a 'hot' radical formed by photolysis of CD_3Br at 185 nm.	RL	298	(9.25±0.65)(-2)			2/2
$\text{CD}_3 + \text{HD} \rightarrow \text{CD}_3\text{H} + \text{D}$ Methyl-d ₃ + Deuterium hydride 72 SHA/WES $k_{\text{ref}}: \text{CD}_3 + \text{DH} \rightarrow \text{CD}_4 + \text{H}.$	RL	398-718	(9.32±1.33)(-1)	0	-275±66	2/2
$\text{CD}_3^* + \text{D}_2 \rightarrow \text{CD}_4 + \text{D}$ Methyl-d ₃ + Deuterium molecule 73 TIN/WES $k_{\text{ref}}: \text{CD}_3^* + \text{H}_2 \rightarrow \text{CD}_4\text{H} + \text{H}.$ CD_3^* is a 'hot' radical formed by photolysis of CD_3Br at 185 nm.	RL	298	(2.15±0.20)			2/2
$\text{CH}_3 + \text{SO}_2 (+ \text{M}) \rightarrow \text{CH}_3\text{SO}_2 (+ \text{M})$ Methyl + Sulfur dioxide 74 JAM/KER Azomethane Flash-photolysis. M = Ar, or N ₂ . P-independent k. P(Total) = (50-200) torr. Same data given in 73 JAM/KER.	EX	298	(1.75±0.25)(11)			2
$\text{CH}_3 + \text{NO} (+ \text{M}) \rightarrow \text{CH}_3\text{NO} (+ \text{M})$ Methyl + Nitrogen oxide (NO) 71 VAN/CAL M = N ₂ , or Propane. Limiting high-pressure k. 72 DAV/COR $k_{\text{ref}}: \text{CH}_3 + \text{NO}_2 \rightarrow \text{CH}_3\text{NO}_2$ 74 TIT/BAL M = (CH ₃) ₂ CO. Limiting high-pressure k. 75 LAU/BAS2 M = He, Ar, N ₂ . Limiting high-pressure k. RRKM fit. 76 PIL/ROB M = Ar, or SF ₆ . RRKM extrapolation of data. Limiting high-pressure k. 74 PRA/VEL M = He. 74 TIT/BAL M = (CH ₃) ₂ CO. Low-pressure k.	EX	295	(1.00±0.15)(13)			2
	RL	295	6.2(-1)			2/2
	EX	443	1.8(12)			2 1.1
	RN	298	1.93(13)			2
	EX	298	(7.23±0.60)(12)			2
	EX	295	(1.0±0.1)(17)			3
	EX	443	6.1(18)			3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
76 PRA/VEL2 M = He. RRKM calculation.	CO	325-521	7.24(16)	0	-211±10	3	1.20
80 WAS CH ₃ generated by reacting O with Ethene. Fast-flow. Photoionization Mass-spectrometry. Comparable data in 79 WAS1, 79 WAS2 and 79 WAS3. P(He) = (1.8-6.3) torr. P(CH ₂ =CH ₂) ₀ = (0.45-0.57) mtorr. P(O) ₀ = (0.15-0.31) mtorr.	EX	298	(8.71±2.90)(17)			3	
CH ₃ + NO ₂ (+ M) → CH ₃ O + NO (+ M) (a) → CH ₃ ONO (+ M) (b) → CH ₃ NO ₂ (+ M) (c)							
Methyl + Nitrogen oxide (NO ₂)							
74 GLA/TRO2 -k _a .	EX	1100-1400	1.3(13)	0	0	2	
81 YAM/SLA k _a . CH ₃ produced by IR Multiphoton dissociation of C ₆ F ₅ OCH ₃ in He. Photoionization Mass-spectrometry. [NO ₂] = (1.10-3.31) × 10 ¹² molec.cm ⁻³ . [CH ₃] ₀ = 1.1 × 10 ¹¹ molec.cm ⁻³ . P(Total) = 1 torr.	EX	295	(1.51±0.30)(13)			2	
72 DAV/COR k _b /k _c .	RL	295	2.17			2/2	
74 GLA/TRO2 ¹⁾ k _c . M = Ar. Estimated, limiting high-pressure k.	RN	300-1400	≈2.07(13)	-0.6	0	2	
74 GLA/TRO2 ¹⁾ k _c . M = Ar. Estimated, low-pressure k. Rate constant expressed as k/[Ar].	RN	300-1400	≈3.58(20)	-6.0	0	3	
¹⁾ Preexponential factor expressed as: A(T/298) ⁿ .							
CH ₃ + N ₂ O → CH ₃ O + N ₂							
Methyl + Nitrogen oxide (N ₂ O)							
73 FAL/HOA	RN	873	(1.4±0.3)(7)			2	
77 BOR/ZAM Estimated, upper-limit k.	ES	1000-2000	<1.0(15)	0	14276	2	
CH ₃ + CO (+ M) → CH ₃ CO (+ M) (a) → CH=CH + OH (+ M) (b)							
Methyl + Carbon monoxide							
74 WAT/WOR k _a .	RN	260-296	1.58(11)	0	3007±12	2	1.58
82 ANA/MAW ¹⁾ k _a . Limiting high-pressure k.	EX	303	9.64(6)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 ANA/MAW ¹⁾ k _a . Limiting high-pressure k.	EX	343	3.43(7)				2
81 PAR ²⁾ k _a . P(CO) = 100 torr.	EX	298	(1.08±0.12)(6)				3
81 PAR ²⁾ k _a . P(CO) = 750 torr.	EX	298	(3.61±0.60)(6)				3
82 ANA/MAW ¹⁾ k _a . Limiting low-pressure k.	EX	303	2.07(12)				3
82 ANA/MAW ¹⁾ k _a . Limiting low-pressure k.	EX	343	3.88(12)				3
81 TSU/KAT k _b . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ behind reflected shock-waves. UV-absorption. IR-emission. Same data given in 81 TSU/HAS.	ES	1500-1900	3.80(13)	0	30432		2
¹⁾ M = CO. Molecular modulation. CH ₃ produced by photolysis of Azoethane. [Azomethane] = 1.0x10 ¹⁷ molec.cm ⁻³ . [CO] = (0.3-2.7)x10 ¹⁹ molec.cm ⁻³ . ²⁾ Photolysis of Acetone at (25.4-40.0) nm. Molecular modulation.							
CH ₃ + CH ₃ (+ M) → CH ₃ CH ₂ + H (+ M) (a) → CH ₂ =CH ₂ + H ₂ (+ M) (b) → CH ₃ CH ₃ (+ M) (c)							
Methyl							
80 ROT/BAR k _a . CH ₃ CH ₃ thermolysis behind shock-waves. Atomic Resonance-Absorption. Computer simulation. Decomposition of CH ₃ CH ₂ to CH ₂ =CH ₂ + H is suggested. Total conc. ~ 4.0x10 ¹⁸ molec.cm ⁻³ . Same data given in 79 ROT/JUS2 and 80 ROT.	DE	2150-1850	8.01(14)	0	13400		2
81 CHI/SKI2 k _a . M = Ar. Ethane pyrolysis behind reflected shock-waves. Resonance-absorption spectroscopy. Decomposition of CH ₃ CH ₂ is suggested. Data-fit. P(Total) = (2-3) atm.	ES	1240-1700	4.0(14)	0	13387		2
78 TSU k _a + k _b . Shock-tube.	EX	1396-2396	9.7(15)	0	15396		2
75 GAR/OWE k _b .	EX	2000-2651	6.0(16)	0	21651		2
71 CLA/IZO1 k _c . Shock-waves. TOF Mass-spectrometry.	EX	1120-1400	(8.4±3.6)(12)	0	0		2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
72 TEN/JON k _c . Data-fit to a proposed mechanism.	CO	303-603	2.63(13)	0	216	2	
73 BAS/LAU k _c . M = He. Limiting high-pressure k.	EX	298	(5.74±0.71)(13)			2	
73 BAY/BRO k _c .	EX	295	(2.4±0.2)(13)			2	
73 TRU/RIC k _c . M = N ₂ . Limiting high-pressure k.	EX	313	(2.41±0.18)(13)			2	
74 JAM/SIM k _c . M = Ar. Limiting high-pressure k.	EX	298	(3.37±0.46)(13)			2	
74 POH/LEI k _c . M = He, or N ₂ , or N ₂ + CO.	EX	298	(2.7±0.3)(13)			2	
76 CAL/MET k _c .	EX	295	(3.31±0.18)(13)			2	
76 GLA/QUA k _c . M = Ar. Limiting high-pressure k. Average k at highest concentrations.	EX	1200-1500	(1.02±0.36)(13)			2	
76 PAR/PAU k _c . M = N ₂ .	EX	250-450	(2.41±0.52)(13)			2	
76 VAN k _c . Extrapolated, limiting high-pressure k.	EX	1350	2.0(13)			2	1.5
77 GLA/QUA k _c . M = Ar. Limiting high-pressure k.	EX	1400	(1.75±0.90)(13)			2	
77 HEL/MAN k _c . Flow-reactor. UV absorption spectroscopy. Limiting high-pressure k. P = (10-80) torr.	ES	1005	1.41(13)			2	
77 HOC/GHO k _c . M = N ₂ . Limiting high-pressure k.	EX	295	(3.1±0.6)(13)			2	
78 PAC/WIM k _c . Neopentane flow-pyrolysis. P = 7.6 torr.	CO	821	2.1(13)			2	
79 SEP/MAR ¹⁾ P(Ar) ~ 14 torr.	EX	750	5.0(12)			2	
79 SEP/MAR ¹⁾ P(Ar) = 7.4 torr.	EX	640-818	3.98(12)			2	
¹⁾ k _c . Discharge-flow. Best-fit.							
79 ZAS/SMI k _c . M = Ar. Tetramethyltin decomposition behind incident and reflected shock-waves. High-pressure k. [Ar] = (0.1-5.5) × 10 ¹⁹ molec.cm ⁻³ .	EX	1750	(1.33±0.66)(13)			2	
80 ADA/BAS2 k _c . Azomethane Flash-photolysis. Absorption spectroscopy.	EX	298	(3.2±0.4)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref)), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
80 BAU/DUX k _c . Recommended high-pressure k. Critical review.	RE	250-420	2.40(13)	0	0	2	1.2
80 PAC/WIM1 k _c . C(CH ₃) ₄ pyrolysis in a flow-reactor. Extrapolated limiting high-pressure k. P = (4-335) torr.	EX	823	(2.2±0.5)(13)			2	
76 VAN ²⁾ k _c . M = He. Extrapolated limiting low-pressure k.	EX	450	2.3(21)			3	4.0
76 VAN ²⁾ k _c . M = He. Calculated limiting low-pressure k.	CO	450	7.4(21)			3	
76 VAN ²⁾ k _c . M = Ar. Extrapolated limiting low-pressure k.	EX	1350	1.2(19)			3	4.0
76 VAN ²⁾ k _c . M = Ar. Calculated limiting low-pressure k.	CO	1350	2.8(19)			3	2.0
²⁾ Rate constants expressed as k/[M].							
CH ₃ [*] + CH ₃ → CH ₄ + CH ₂							
Methyl							
77 RIC/TRU Upper-limit k. M = Ar. CH ₃ [*] is an energy-rich radical formed by photolysis of CH ₃ I at 260 nm.	EX	298	≤1.02(14)			2	
CD ₃ + CD ₃ (+ M) → CD ₂ =CD ₂ + D + D (+ M) (a) → CD ₃ CD ₃ (+ M) (b)							
Methyl-d ₃							
81 CHI/SKI2 k _a . M = Ar. Ethane pyrolysis behind reflected shock-waves. Resonance-absorption. Data-fit to a proposed mechanism. P(Total) = (2-3) atm.	ES	1240-1700	4.0(14)	0	13387	2	
76 CAL/MET k _b . M = N ₂ .	EX	295	(2.95±0.24)(13)			2	
76 GLA/QUA k _b . M = Ar. Limiting high-pressure k. Average k at highest concentrations.	EX	1200-1500	(1.33±0.54)(13)			2	
76 PAR/PAU k _b . M = N ₂ .	EX	298	(2.41±0.52)(13)			2	
77 GLA/QUA k _b . M = Ar. Limiting high-pressure k.	EX	1400	(1.93±1.02)(13)			2	
76 VAN k _b . M = Ar. Extrapolated limiting low-pressure k.	EX	1350	7.0(19)			3	4.0
76 VAN k _b . M = Ar. Calculated limiting low-pressure k.	CO	1350	7.7(19)			3	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
$\text{CH}_3 + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_3 + \text{H}$ (a)						
$\rightarrow \text{CH}_3\text{CH}_2 + \text{H}_2$ (b)						
Methyl + Methane						
79 TAB/BAU ¹⁾	ES	1950-2770	8.0(13)	0	20131	2
k_a .						
79 TAB/BAU ¹⁾	ES	1950-2770	1.0(13)	0	11576	2
k_b .						
¹⁾ M = Ar. Methane pyrolysis in shock-waves. Best data-fit on the basis of a proposed mechanism.						
Total conc.: $(1.4-5.4) \times 10^{18}$ molec.cm ⁻³ .						
$\text{CH}_3 + \text{CHO} \rightarrow \text{CH}_4 + \text{CO}$ (a)						
$\rightarrow \text{CH}_3\text{CHO}$ (b)						
Methyl + Methyl, oxo-						
77 HEL/MAN	ES	1005	3.78(13)			2
k_a . Pyrolysis in a flow-reactor. Absorption-spectroscopy. Gas-chromatography.						
P = (10-80) torr.						
79 NAD/SAR4	EX	298	>3.01(13)			2
k_a . Intracavity laser spectroscopy. Lower-limit k.						
80 MUL	EX	298	(2.66±0.97)(13)			2
k_b . CH ₃ CHO decomposition by pulsed UV-Photolysis. Internal-resonator Laser-Spectroscopy.						
79 NAD/SAR2	EX	298	(1.39±0.60)(14)			2
k_{overall} . Pulse-photolysis of CH ₃ CHO.						
$\text{CH}_3 + \text{HCHO} \rightarrow \text{CH}_4 + \text{CHO}$						
Methyl + Formaldehyde						
77 HEL/MAN	ES	1005	3.16(10)			2
Pyrolysis in a flow-reactor. UV-Absorption-spectroscopy. Gas-chromatography.						
P = (10-80) torr.						
$\text{CH}_3 + \text{CH}_3\text{O} \rightarrow \text{CH}_4 + \text{HCHO}$ (a)						
$\rightarrow \text{CH}_3\text{OCH}_3$ (b)						
Methyl + Methoxy						
79 HAS/KOS ¹⁾	RN	298	2.71(13)			2
k_a .						
79 HAS/KOS ¹⁾	RN	298	3.31(13)			2
k_b .						
¹⁾ Flash-photolysis of CH ₃ COOCH ₃ . k's determined relative to the reaction: $\text{CH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_3$.						
P = (1.5-700) torr. Gas-chromatography.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{O} + \text{CH}_3\text{O}$ Methyl + Methylendioxy							
77 PAR	EX	298	(3.61±0.60)(13)			2	
$\text{CD}_3 + \text{COS} \rightarrow \text{CD}_3\text{S} + \text{CO}$ Methyl-d ₃ + Carbon oxide sulfide							
72 JAK/AHM	RN	354-490	3.80(11)	0	5712±176	2	1.78
$\text{CH}_3 + \text{CH}_3\text{N}=\text{NH} \rightarrow \text{CH}_4 + \text{CH}_3\text{N}=\text{N}$ Methyl + Diazene, methyl-							
76 VID/WIL	EX	294	(1.31±0.17)(10)			2	
$\text{CH}_3 + \text{CH}_3\text{NO}_2 \rightarrow \text{CH}_4 + \text{CH}_2\text{NO}_2$ Methyl + Methane, nitro-							
80 BAL/FED Continuous-circulation Molybdenum glass-reactors. Gas-chromatography. P(Total) = (126-133) torr.	EX	413-482	7.07(11)	0	5606±282	2	1.95
$\text{CH}_3 + \text{CH}=\text{CH} \rightarrow \text{CH}_3\text{CH}=\text{CH}$ Methyl + Ethyne							
77 HOL/KER	RN	379-487	6.19(11)	0	3875±755	2	6.31
$\text{CH}_3 + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_4 + \text{CH}_2=\text{CH} \text{ (a)}$ $\quad \quad \quad \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2 \text{ (b)}$ Methyl + Ethene							
76 CHE/BAC k_a .	RN	1038	1.0(9)			2	
79 TAB/BAU k_a . M = Ar. CH_4 pyrolysis in shock-waves. Best data-fit. Total conc.: (1.4-5.4)×10 ¹⁸ molec.cm ⁻³ .	EX	1950-2770	5.0(12)	0	6543	2	
72 TED/WAL ¹⁾ k_{ref} : $\text{CH}_3 + \text{CH}_2=\text{CHF} \rightarrow \text{CH}_3\text{CH}_2\text{CHF}$	RL	335-424	7.24(2)	0	-468±101	2/2	1.07
72 TED/WAL ¹⁾ k_{ref} : $\text{CH}_3 + \text{CH}_2=\text{CF}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CF}_2$	RL	335-424	4.90(1)	0	-2416±503	2/2	1.23
72 TED/WAL ¹⁾ k_{ref} : $\text{CH}_3 + \text{CF}_2=\text{CF}_2 \rightarrow \text{CH}_3\text{CF}_2\text{CF}_2$	RL	335-424	8.32(3)	0	1319±554	2/2	1.23
72 TED/WAL ¹⁾ k_{ref} : $\text{CH}_3 + \text{CH}_2=\text{CHCl} \rightarrow \text{CH}_3\text{CH}_2\text{CHCl}$	RL	335-424	2.88(2)	0	-941±252	2/2	1.10
72 TED/WAL ¹⁾ k_{ref} : $\text{CH}_3 + \text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CHCH}_3$ ¹⁾ k_b/k_{ref} .	RL	335-424	1.07(4)	0	-377±201	2/2	1.07

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 CAM/MAR k _b . Determined from k _{-b} and thermochemical data.	DE	676-813	3.16(10)	0	3969	2	
77 HOL/KER k _b .	RN	350-503	2.09(11)	0	3674±503	2	3.16
CH₃ + CH₃CH₂ → CH₃CH₂CH₃							
Methyl + Ethyl							
72 TEN/JON	CO	303-603	2.51(13)	0	201	2	
75 LIF/FRE1 k ₁ = k ₋₁ K.	DE	1050-1250	2.4(12)			2	
80 KOI/GAR Propane Thermolysis behind reflected shock-waves. Absorption Spectroscopy. Data-fit to a proposed mechanism.	ES	1300-1700	7.24(12)	0	0	2	
82 SIM/GAR ¹⁾ 4.3% Propane in Ar. Conc. = 6.0x10 ¹⁸ molec.cm ⁻³ .	ES	1300-1700	8.0(10)	0	-5700	2	
82 SIM/GAR ¹⁾ 5% Propane in Ar. Conc. = 9.0x10 ¹⁸ molec.cm ⁻³ .	ES	1300-1700	9.0(7)	0	-14700	2	
¹⁾ Pyrolysis of Propane in Ar behind reflected shock-waves. Data-fit to a proposed mechanism.							
CH₃ + CH₃CH₃ → CH₄ + CH₃CH₂							
Methyl + Ethane							
71 CLA/IZO1 Shock-waves. Time-of-flight Mass-spectrometry.	ES	1485	3.55(11)			2	
72 PAC/PUR2	EX	920-1040	5.01(14)	0	10826±2406	2	10.
73 CLA/DOV1 BEBO calculation. The preexponential factor expressed as: A(T/298) ^{4.0} .	CO	300-1800	4.34(9)	4.0	4167±15	2	1.02
74 YAM/RYP	RN	980-1130	3.02(12)	0	6844±1107	2	3.16
76 BRA/WES2 Computer simulation optimization.	DE	1055-1325	3.24(13)	0	9057	2	1.78
76 CHE/BAC k for α ~ 1. Measured k values also given at T = 880, 995 and 1068 K. Non-Arrhenius behaviour.	EX	1038	(1.3±0.3)(10)			2	
77 HEL/MAN Flow-reactor pyrolysis. Absorption spectroscopy. Gas-chromatography. P = (10-80) torr.	ES	1005	3.98(9)			2	
79 ROT/JUS2 Shoch-tube. Atomic Resonance-absorption Spectrophotometry. k determined by computer simulation. Total conc. = (0.2-2.3)x10 ¹⁹ molec.cm ⁻³ .	DE	1450-1600	5.00(13)	0	9800	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3 + \text{CH}_3\text{CO} \rightarrow \text{CH}_4 + \text{CH}_2=\text{C}=\text{O}$ (a)						
$\rightarrow \text{CH}_3\text{CH}_3 + \text{CO}$ (b)						
$\rightarrow (\text{CH}_3)_2\text{CO}$ (c)						
Methyl + Ethyl, 1-oxo- (Acetyl)						
78 ADA/BAS	ES	298	7.5(13)			2
$k_a + k_b + k_c$. Acetone Flash-photolysis						
Kinetic Spectroscopy.						
P(Total) = 50 torr.						
81 ADA/BAS2	ES	298	8.6(13)			2
$k_a + k_b + k_c$. Acetone Flash-photolysis.						
Kinetic Spectroscopy.						
81 ADA/BAS2	RL	298	3.8(-1)			2/2
$k_b/(k_a + k_b + k_c)$. Acetone Flash-photolysis.						
Kinetic-Spectroscopy. Estimated ratio.						
79 HAS/KOS	RN	298	3.30(13)			2
k_c . Flash-photolysis of $\text{CH}_3\text{COOCH}_3$. k determined						
relative to the reaction: $\text{CH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_3$.						
Gas-chromatography.						
P = (1.5-700) torr.						
82 ANA/MAW	RN	263-343	(2.26±0.27)(13)	0	0	2
k_c . Average of 24 k values obtained through						
data-fit. Molecular Modulation Spectroscopy. CH_3						
and CH_3CO produced by photolysis of Azomethane						
in presence of CO. Gas-chromatography. P-inde-						
pendent k. [Azomethane] = 1.0×10^{17} molec.cm ⁻³ .						
[CO] = $(0.3-2.7) \times 10^{19}$ molec.cm ⁻³ .						
82 TIM/KAL	EX	298	(2.98±0.17)(13)			2
k_c . Flash-photolysis of 2,3-Butanedione.						
Gas-chromatography.						
$[\text{CH}_3] = (0.26-6.08) \times 10^{18}$ molec.cm ⁻³ .						
$[\text{CH}_3\text{CO}] = (1.14-5.77) \times 10^{18}$ molec.cm ⁻³ .						
P = (11-47) torr.						
$\text{CD}_3 + \text{CD}_3\text{CO} \rightarrow \text{CD}_4 + \text{CD}_2=\text{C}=\text{O}$ (a)						
$\rightarrow \text{CD}_3\text{CD}_3 + \text{CO}$ (b)						
$\rightarrow (\text{CD}_3)_2\text{CO}$ (c)						
Methyl-d ₃ + Ethyl-2,2,2-d ₃ -1-oxo- (Acetyl-d ₃)						
81 ADA/BAS2	ES	298	5.2(13)			2
$k_a + k_b + k_c$. Acetone-d ₆ Flash-photolysis.						
Kinetic Spectroscopy.						
81 ADA/BAS2	RL	298	4.7(-1)			2/2
$k_b/(k_a + k_b + k_c)$. Acetone-d ₆ Flash-photolysis.						
Kinetic-Spectroscopy. Estimated ratio.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3 + \text{CH}_3\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CO}$ (a) $\rightarrow \text{CH}_4 + \text{CH}_2\text{CHO}$ (b) $\rightarrow (\text{CH}_3)_2\text{CHO}$ (c)						
Methyl + Acetaldehyde						
71 BAL/LAN k_a .	ES	713-813	(1.6±0.6)(12)	0	4127±252	2
75 COL/NAE k_b .	ES	800-1225	4.37(15)	0	14570	2
76 BAR/BER $(k_a + k_b)/k_{\text{ref}}$ $k_{\text{ref}}: \text{CH}_3 + \text{CH}_3\text{CDO} \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{CO}$	RL	785	2.7			2/2
75 BAT/MCC k_c .	ES	393-473	7.94(10)	0	0±503	2
$\text{CH}_3 + \text{CH}_3\text{CDO} \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{CO}$ (a) $\rightarrow \text{CH}_4 + \text{CH}_2\text{CDO}$ (b)						
Methyl + Acetaldehyde-1-d						
76 BAR/BER k_b/k_a .	RL	785	6.2(-1)			2/2
$\text{CH}_3 + \text{HC}(\text{O})\text{OCH}_3 \rightarrow \text{CH}_4 + \text{C}(\text{O})\text{OCH}_3$ (a) $\rightarrow \text{CH}_4 + \text{HC}(\text{O})\text{OCH}_2$ (b)						
Methyl + Formic acid methyl ester (Methyl formate)						
71 DON/DOR ¹⁾	EX	400-513	5.01(11)	0	5184±101	2 1.26
71 DON/DOR ¹⁾	EX	455	5.62(6)			2
¹⁾ $k_a + k_b$. Acetone photolysis. Mass-spectrometry.						
$\text{CD}_3 + \text{HC}(\text{O})\text{OCH}_3 \rightarrow \text{CD}_3\text{H} + \text{C}(\text{O})\text{OCH}_3$ (a) $\rightarrow \text{CD}_3\text{H} + \text{HC}(\text{O})\text{OCH}_2$ (b)						
Methyl-d ₃ + Formic acid methyl ester (Methyl formate)						
71 DON/DOR ¹⁾	EX	400-513	3.55(11)	0	5033±252	2 1.74
71 DON/DOR ¹⁾	EX	455	5.25(6)			2
¹⁾ k_a . Acetone photolysis. Mass-spectrometry.						
71 DON/DOR ²⁾	EX	400-513	4.37(11)	0	5083±151	2 1.38
71 DON/DOR ²⁾	EX	455	6.17(6)			2
¹⁾ $k_a + k_b$. Acetone photolysis. Mass-spectrometry.						
$\text{CD}_3 + \text{DC}(\text{O})\text{OCH}_3 \rightarrow \text{CD}_4 + \text{C}(\text{O})\text{OCH}_3$ (a) $\rightarrow \text{CD}_3\text{H} + \text{DC}(\text{O})\text{OCH}_2$ (b)						
Methyl-d ₃ + Formic-d acid methyl ester (Methyl formate-d)						
71 DON/DOR ¹⁾	EX	400-513	3.02(11)	0	5888±151	2 1.45
71 DON/DOR ¹⁾	EX	455	6.92(5)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
1) k_a . Acetone photolysis. Mass-spectrometry.							
71 DON/DOR ²⁾	EX	400-513	1.23(11)	0	5435±101	2	1.29
71 DON/DOR ²⁾	EX	455	7.59(5)			2	
2) k_b . Acetone photolysis. Mass-spectrometry.							
1) Photolysis of Acetone. Mass-spectrometry.							
$\text{CH}_3 + (\text{CH}_3)_2\text{O} \rightarrow \text{CH}_4 + \text{CH}_2\text{OCH}_3$							
Methyl + Methane, oxybis- (Dimethyl ether)							
75 PAC	EX	782-936	3.16(13)	0	7578±842	2	2.51
Curved Arrhenius plot over the extended T-range (373-936) K.							
77 HEL/MAN	ES	1005	1.31(10)			2	1.58
Pyrolysis in a flow-reactor. UV-Absorption spectroscopy. Gas-chromatography. P = (10-80) torr.							
82 BAT/ALV ¹⁾	EX	373-473	2.00(11)	0	4781±101	2	1.26
82 BAT/ALV ¹⁾	SE	373-935	3.55(12)	0	5939±101	2	1.26
Extended T-range by combining the above k with data found in the literature.							
1) Photolysis of Azomethane in the presence of Dimethyl ether. $P(\text{CH}_3\text{OCH}_3) = (0-470)$ torr. $P(\text{Azomethane}) = 23$ torr.							
$\text{CH}_3 + \triangle \rightarrow \text{CH}_3\text{S} + \text{CH}_2=\text{CH}_2$							
Methyl + Thiirane (Ethylene episulfide)							
72 JAK/AHM	RN	304-478	7.08(10)	0	3372±403	2	3.02
$\text{CD}_3 + \triangle \rightarrow \text{CD}_3\text{H} + \triangle$ (a)							
$\rightarrow \text{CD}_3\text{S} + \text{CH}_2=\text{CH}_2$ (b)							
Methyl-d ₃ + Thiirane (Ethylene episulfide)							
72 JAK/AHM	RN	303-477	2.19(11)	0	4801±503	2	3.98
k_a .							
72 JAK/AHM	RN	303-477	5.89(10)	0	3271±554	2	4.37
k_b .							
$\text{CH}_3 + (\text{CH}_3)_2\text{S} \rightarrow \text{CH}_4 + \text{CH}_3\text{SCH}_2$							
Methyl + Methane, thiobis- (Dimethyl sulfide)							
76 ART/LEE	RN	393-518	4.17(11)	0	4613±82	2	1.20

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3 + \text{CH}_3\text{N}=\text{NCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{N}=\text{NCH}_2$							
Methyl + Diazene, dimethyl- (Azomethane)							
77 SCH/KNO	RL	524-565	1.0	0	-604±302	2/2	2.0
$k_{\text{ref}}: \text{CH}_3 + \text{CD}_3\text{COCOCOD}_3 \rightarrow \text{CH}_3\text{D} + \text{CD}_3\text{COCOCOD}_3$							
80 DUR/MAR	EX	323-453	1.07(12)	0	4906±132	2	1.41
Photolysis of 14% Azomethane in Propane at 366 nm. P = (25-300) torr.							
$\text{CD}_3 + \text{CH}_3\text{N}=\text{NCH}_3 \rightarrow \text{CD}_3\text{H} + \text{CH}_2\text{N}=\text{NCH}_3$							
Methyl-d ₃ + Diazene, dimethyl- (Azomethane)							
77 SCH/KNO	RL	524-565	6.3(-1)	0	-755±302	2/2	2.0
$k_{\text{ref}}: \text{CD}_3 + \text{CD}_3\text{COCOCOD}_3 \rightarrow \text{CD}_4 + \text{CD}_2\text{COCOCOD}_3$							
$\text{CH}_3 + \text{CH}_2=\text{C}=\text{CH}_2 \rightarrow \text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$							
Methyl + 1,2-Propadiene (Allene)							
73 TSA2	ES	996-1180	1.58(11)	0	2500	2	
1100 K given by the author as central T.							
$\text{CH}_3 + (\text{CH}_3)_2\text{CH} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}=\text{CH}_2$ (a)							
$\rightarrow (\text{CH}_3)_3\text{CH}$ (b)							
Methyl + Ethyl, 1-methyl- (Isopropyl)							
72 ARI/STE	RL	295	(2.4±0.3)(-1)			2/2	
k_a/k_b . Azoisopropane photolysis.							
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2$ (a)							
$\rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CH}$ (b)							
Methyl + Propane							
75 CAM/MAR	EX	676-743	2.00(12)	0	5689±818	2	3.31
$k_a + k_b$. Low-T region.							
75 CAM/MAR	EX	743-813	5.01(15)	0	11595±902	2	3.24
$k_a + k_b$. High-T region.							
75 LIF/FRE1	EX	1050-1250	3.55(12)	0	5184	2	
$k_a + k_b$. Data-fit to a proposed mechanism.							
79 PRA/ROG2	ES	1008	(4.2±1.1)(9)			2	
$k_a + k_b$. M = Ar. Propane pyrolysis in a wall-less reactor. Average k at the mean experimental T. Other k values within the 967-1051 K T-range are also given. Approximate fit. P(Ar) = 600 torr.							
80 DUR/MAR	RN	323-453	2.6(11)	0	4896±132	2	1.41
$k_a + k_b$. Photolysis of 14% Azomethane in Propane at 366 nm. P = (25-300) torr. k determined relative to the reaction: $\text{CH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_3$							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 HAU/SAN $k_a + k_b$. Pyrolysis in a flow-reactor. The preexponential factor expressed as: $A(T/298)^n$.	EX	1110-1235	6.23(9)	4.0	4177	2	
$\text{CH}_3 + \text{CH}_3\text{C}(\text{O})\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CO} + \text{CO}$ Methyl + Propanal, 2-oxo-							
77 KYL/ORC	RN	353-444	1.38(11)	0	3332±337	2	2.40
$\text{CH}_3 + (\text{CH}_3)_2\text{CO} \rightarrow \text{CH}_4 + \text{CH}_2\text{C}(\text{O})\text{CH}_3$ (a) $\rightarrow (\text{CH}_3)_3\text{CO}$ (b) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{O}$ (c) Methyl + 2-Propanone							
72 SHA/WES k_a/k_{ref} . k_{ref} : $\text{CH}_3 + \text{D}_2 \rightarrow \text{CH}_3\text{D} + \text{D}$.	RL	398-718	(6.17±0.46)(-1)	0	-1021±38	2/2	
72 SHA/WES k_a/k_{ref} . k_{ref} : $\text{CH}_3 + \text{DH} \rightarrow \text{CH}_3\text{D} + \text{H}$.	RL	398-718	(2.3±0.92)	0	-413±186	2/2	
76 ART/LEE k_a .	RN	393-518	4.07(11)	0	4869±55	2	1.12
79 ART/NEW1 k_a . Acetone photolysis.	EX	117-244	3.39(11)	0	4882±20	2	1.05
71 CAD/TRO k_b . $k_b = k_{-b}K$.	DE	373-423	1.74(9)	0	6772±902	2	10.0
80 KNO/RIC k_b . Thermolysis of Azomethane and di-t-Butyl peroxide. Mass-spectrometry. k determined relative to reaction: $\text{CH}_3 + (\text{CD}_3)_2\text{CO} \rightarrow \text{CH}_3\text{D} + \text{CD}_2\text{C}(\text{O})\text{CD}_3$	RN	413-563	3.16(10)	0	5788±554	2	2.51
75 BAT/MCC k_c .	ES	393-473	2.0(11)	0	0±503	2	
$\text{CH}_3 + (\text{CD}_3)_2\text{CO} \rightarrow \text{CH}_3\text{D} + \text{CD}_2\text{C}(\text{O})\text{CD}_3$ (a) $\rightarrow (\text{CD}_3)_2\text{C}(\text{CH}_3)\text{O}$ (b) Methyl + 2-Propanone-1,1,1,3,3,3-d ₆							
80 KNO/RIC ¹⁾ k_a/k_b .	RL	413-563	1.48(1)	0	-151±86	2/2	1.17
80 KNO/RIC ¹⁾ k_b .	RN	413-563	3.16(10)	0	5888±252	2	1.59
¹⁾ Thermolysis of Azomethane and di-t-Butyl peroxide.							
$\text{CD}_3 + (\text{CD}_3)_2\text{CO} \rightarrow \text{CD}_4 + \text{CD}_3\text{C}(\text{O})\text{CD}_2$ Methyl-d ₃ + 2-Propanone-1,1,1,3,3,3-d ₆							
72 SHA/WES k_{ref} : $\text{CD}_3 + \text{H}_2 \rightarrow \text{CD}_3\text{H} + \text{H}$	RL	398-718	(8.56±0.68)(-1)	0	532±36	2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
72 SHA/WES $k_{\text{ref}}: \text{CD}_3 + \text{HD} \rightarrow \text{CD}_3\text{H} + \text{D}$	RL	398-718	(1.47±0.13)	0	340±42	2/2	
$\text{CH}_3 + \text{CH}_3\text{C}(\text{O})\text{OCH}_3 \rightarrow \text{CH}_4 + \text{CH}_2\text{C}(\text{O})\text{OCH}_3$ (a) $\rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{O})\text{OCH}_2$ (b) Methyl + Acetic acid methyl ester (Methyl acetate)							
79 ART/NEW2 ¹⁾ k_a .	EX	389-497	1.48(11)	0	5160±212	2	1.66
79 ART/NEW2 ¹⁾ k_b .	EX	389-497	2.75(11)	0	5651±155	2	1.45
79 ART/NEW2 ¹⁾ $k_a + k_b$.	EX	389-497	3.63(11)	0	5344±117	2	1.32
¹⁾ Photolysis in silica vessel.							
$\text{CH}_3 + \text{CH}_3\text{C}(\text{O})\text{OCD}_3 \rightarrow \text{CH}_4 + \text{CH}_2\text{C}(\text{O})\text{OCD}_3$ (a) $\rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{C}(\text{O})\text{OCD}_2$ (b) Methyl + Methan-d ₃ -ol acetate (Methyl-d ₃ acetate)							
81 ART/NEW ¹⁾ k_a .	EX	386-505	2.04(11)	0	5232±124	2	1.32
81 ART/NEW ¹⁾ k_b .	EX	386-505	2.14(11)	0	6430±77	2	1.20
¹⁾ Photolysis in silica vessel.							
$\text{CH}_3 + \text{CD}_3\text{C}(\text{O})\text{OCH}_3 \rightarrow \text{CH}_3\text{D} + \text{CD}_2\text{C}(\text{O})\text{OCH}_3$ (a) $\rightarrow \text{CH}_4 + \text{CD}_3\text{C}(\text{O})\text{OCH}_2$ (b) Methyl + Acetic acid-d ₃ methyl ester (Methyl acetate-d ₃)							
79 ART/NEW2 k_a . Photolysis in silica vessel.	EX	389-497	2.45(11)	0	6268±40	2	1.10
$\text{CH}_3 + \text{H}_3\text{C} \begin{array}{c} \text{S} \\ \diagup \diagdown \end{array} \rightarrow \text{CH}_3\text{S} + \text{CH}_3\text{CH}=\text{CH}_2$ (a) $\rightarrow \text{CH}_4 + [\text{C}_3\text{H}_5\text{S}]$ (b) Methyl + Thiirane, methyl-							
72 JAK/AHM k_a .	RN	339-435	2.14(11)	0	3749±835	2	8.32
72 JAK/AHM k_b .	RN	339-435	1.0(11)	0	4157±438	2	3.02

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3 + (\text{CH}_3)_2\text{CHNO}_2 \rightarrow \text{CH}_4 + \text{CH}_2\text{CH}(\text{CH}_3)\text{NO}_2$ (a)							
$\rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CNO}_2$ (b)							
Methyl + Propane, 2-nitro-							
77 BAL/TIT ¹⁾	EX	413-479	1.38(11)	0	4222±257	2	1.74
78 TIT/BAL ¹⁾	EX	413-479	1.26(11)	0	4227±252	2	2.0
¹⁾ $k_a + k_b$.							
Flow-reactor.							
P(Total) 100 torr.							
$\text{CH}_3 + \text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$							
Methyl + 2-Propenyl, 2-methyl-							
73 TSA2	EX	996-1180	2.0(13)			2	
1020 K given by the author as central-T.							
$\text{CH}_3 + \text{trans-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_4 + \text{CH}_2\text{CH}=\text{CHCH}_3$							
Methyl + 2-Butene, (Z)-							
73 RIC/MAR	RL	768	≈8.0			2/2	
$k_{\text{ref}}:$							
$\text{CH}_3 + \text{CH}_3\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CO}$							
$\text{CH}_3 + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow \text{CH}_4 + \text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$							
Methyl + 1-Propene, 2-methyl-							
73 KON/MAR	ES	770-855	1.12(14)	0	8858	2	
73 RIC/MAR	RL	768	≈5.0			2/2	
$k_{\text{ref}}:$							
$\text{CH}_3 + \text{CH}_3\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CO}$							
76 BRA/WES1 ¹⁾	EX	1030-1300	2.6(16)	0	13352	2	6.61
76 BRA/WES2 ¹⁾	DE	1055-1325	6.8(13)	0	9803	2	1.62
¹⁾ Computer data-fit to a proposed mechanism.							
80 PAC/WIM1	EX	823	2.2(9)			2	
Neopentane Pyrolysis.							
P = (4-335) torr.							
$\text{CH}_3 + (\text{CH}_3)_3\text{C} \rightarrow (\text{CH}_3)_4\text{C}$							
Methyl + Ethyl, 1,1-dimethyl- (t-Butyl)							
76 MAR/PUR	DE	756-845	7.9(12)	0	0	2	
Estimated k. Computer-fit of data.							
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$ (a)							
$\rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CHCH}_3$ (b)							
Methyl + Butane							
75 YAM	ES	980-1060	5.01(11)	0	6844	2	
k_a .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
72 PAC/PUR1 ¹⁾ Calculation based on experimental data.	DE	869-952	2.51(14)	0	9160±1610	2 6.31
74 HUG/MAR ¹⁾ Calculation based on experimental data.	DE	895-981	3.16(13)	0	7434±1804	2 7.94
75 YAM ¹⁾	RN	980-1060	3.16(12)	0	5586±1007	2 2.57
76 YAM/NAM ¹⁾	EX	980-1060	3.16(12)	0	5586±1007	2 2.57
¹⁾ k _a + k _b .						
75 YAM k _b .	ES	980-1060	4.26(11)	0	5284	2
 $\text{CH}_3 + (\text{CH}_3)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHCH}_2$ (a) $\rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{C}$ (b)						
Methyl + Propane, 2-methyl- (i-Butyl)						
73 KON/MAR k _a .	ES	770-855	1.45(13)	0	8203	2
82 SHE/GUS ¹⁾ (k _a + k _b)/k _{ref} . Average ratio. k _{ref} : $\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2$ (c) $\rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CH}$ (d)	RL	1023-1123	(2.2±0.2)			2/2
73 KON/MAR k _b .	ES	770-855	3.24(12)	0	6492	2
82 SHE/GUS ¹⁾ k _b /k _a . Recalculated from a reported tertiary per primary bond rate constant ratio of 10.5 ¹⁾ Propane/Isobutane pyrolysis. P = 100 torr.	RL	1023-1123	1.17			2/2
 $\text{CH}_3 + \text{CH}_3\text{C}(\text{O})\text{C}(\text{O})\text{CH}_3 \rightarrow (\text{CH}_3)_2\text{CO} + \text{CH}_3\text{CO}$ (a) $\rightarrow \text{CH}_4 + \text{CH}_2\text{C}(\text{O})\text{C}(\text{O})\text{CH}_3$ (b) $\rightarrow (\text{CH}_3)_2\text{C}(\text{O}^\cdot)\text{COCH}_3$ (c)						
Methyl + 2,3-Butanedione (Biacetyl)						
73 KNO/SCH k _a . Estimation based on some experimental data.	ES	240-277	2.51(10)	0	3221	2
75 SCH/PLA k _a .	RN	822-905	1.58(11)	0	4328	2
73 KNO/SCH k _b . Estimation based on some experimental data.	ES	240-277	3.16(11)	0	4177	2
75 SCH/PLA k _b .	RN	822-905	7.94(11)	0	4731	2
75 SCH/PLA k _b /k _a .	RL	822-905	5.01	0	403±755	2 63.1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 SCH/KNO k_b/k_{ref} k_{ref} : $CH_3 + CD_3C(O)C(O)CD_3 \rightarrow CH_3D + CD_3C(O)C(O)CD_2$	RL	524-565	3.16	0	-302±428	2/2	3.16
78 KNO/SCH ¹⁾ k_b/k_c	RL	655-690	1.58(1)	0	1107±352	2/2	1.58
78 KNO/SCH ¹⁾ k_c	RN	655-690	2.0(10)	0	3070±503	2	2.51
¹⁾ Thermolysis. Gas-chromatography.							
$CH_3 + CD_3C(O)C(O)CD_3 \rightarrow CD_3CO + CH_3C(O)CD_3$ (a) $\rightarrow CD_3 + CH_3C(O)C(O)CD_3$ (b) $\rightarrow CH_3D + CD_2C(O)C(O)CD_3$ (c)							
Methyl + 2,3-Butanedione-1,1,1,4,4,4-d ₆ (Biacetyl-d ₆)							
77 SCH/KNO k_a/k_{ref} k_{ref} : $CD_3 + CD_3C(O)C(O)CD_3 \rightarrow CD_3CO + CD_3C(O)CD_3$	RL	524-565	5.0(-1)	0	604±403	2/2	2.51
77 SCH/KNO k_b/k_a	RL	524-565	3.16	0	3120±453	2/2	2.51
77 SCH/KNO k_c	RN	524-565	7.94(10)	0	7529±377	2	2.51
$CD_3 + CH_3C(O)C(O)CH_3 \rightarrow CD_3H + CH_2C(O)C(O)CH_3$							
Methyl-d ₃ + 2,3-Butanedione (Biacetyl)							
77 SCH/KNO k_{ref} : $CD_3 + CD_2HC(O)C(O)CD_3$ $\rightarrow CD_3H + CD_2C(O)C(O)CD_3$	RL	524-565	1.26	0	-906±101	2/2	1.26
$CD_3 + CD_2HC(O)C(O)CD_3 \rightarrow CD_2HC(O)D_3 + CD_3CO$							
Methyl-d ₃ + 2,3-Butanedione-1,1,1,4,4-d ₅ (Biacetyl-d ₅)							
77 SCH/KNO k_{ref} : $CD_3 + CD_3C(O)C(O)CD_3 \rightarrow CD_3CO + CD_3C(O)CD_3$	RL	660-685	2.0(-1)	0	-906±151	2/2	1.58
$CD_3 + CD_3C(O)C(O)CD_3 \rightarrow CD_4 + CD_2C(O)C(O)CD_3$ (a) $\rightarrow CD_3CO + (CD_3)_2CO$ (b)							
Methyl-d ₃ + 2,3-Butanedione-1,1,1,4,4,4-d ₆ (Biacetyl-d ₆)							
77 SCH/KNO k_a/k_{ref} k_{ref} : $CD_3 + CD_2HC(O)C(O)CD_3$ $\rightarrow CD_3H + CD_2C(O)C(O)CD_3$	RL	660-685	3.98	0	906±101	2/2	1.26
77 SCH/KNO k_a/k_b	RL	660-685	1.0(1)	0	1359±302	2/2	1.58

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 SCH/KNO k_a .	RN	660-685	1.26(11)	0	4680±377	2	2.51
77 SCH/KNO k_b .	RN	660-685	1.26(10)	0	3322±503	2	3.98
$\text{CH}_3 + \text{CH}_3\text{C}(\text{O})\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_2\text{C}(\text{O})\text{CH}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{O})\text{CH}_2\text{CH}_2$ (b) $\rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{O})\text{CHCH}_3$ (c) $\rightarrow (\text{CH}_3)_2\text{C}(\text{O}^\cdot)\text{CH}_2\text{CH}_3$ (d)							
Methyl + 2-Butanone							
80 KNO ¹⁾ $(k_a + k_b + k_c)/k_d$.	RL	563	(4.95±1.90)(2)			2/2	
80 KNO ¹⁾ k_d .	RN	563	2.00(5)			2	2.51
¹⁾ Azomethane-sensitized decomposition.							
$\text{CH}_3 + \text{CD}_3\text{C}(\text{O})\text{CD}_2\text{CH}_3 \rightarrow \text{CH}_3\text{D} + \text{CD}_2\text{C}(\text{O})\text{CD}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_3\text{D} + \text{CD}_3\text{C}(\text{O})\text{CDCH}_3$ (b)							
Methyl + 2-Butanone-1,1,1,3,3-d ₅							
74 SCH/DRE $k_a + k_b$.	RN	523-563	1.26(11)	0	4504±277	2	2.58
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2$ (b) $\rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CHCH}=\text{CH}_2$ (c) $\rightarrow \text{CH}_4 + \text{CH}_3\text{CHCH}_2\text{CH}=\text{CH}_2$ (d) $\rightarrow \text{CH}_4 + \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ (e)							
Methyl + 1-Pentene							
74 SHI/AMA $(k_a + k_b)/(k_c + k_d + k_e)$.	RL	923	1.0			2/2	
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CHCH}(\text{CH}_3)_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CHCH}_3$ (b) $\rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_2$ (c) $\rightarrow \text{CH}_4 + \text{CH}_3\text{CHCH}=\text{CHCH}_3$ (d) $\rightarrow \text{CH}_4 + \text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3$ (e)							
Methyl + 2-Pentene (Unspecified form)							
74 SHI/AMA $(k_a + k_b)/(k_c + k_d + k_e)$.	RL	923	2.0(-1)			2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3 + \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)\text{CH}_2$ (a) $\rightarrow \text{CH}_4 + \text{CH}_3\text{CHC}(\text{CH}_3)=\text{CH}_2$ (b) $\rightarrow \text{CH}_4 + \text{CH}_2\text{CH}=\text{C}(\text{CH}_3)_2$ (c)						
Methyl + 2-Butene, 2-methyl-						
75 BUL/MAR $k_a + k_b$. Static system pyrolysis.	ES	667-770	5.01(13)	0	7578	2
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$						
Methyl + Pentyl						
71 WAT Lower-limit estimate. k_{ref} : $\text{CH}_3 + \text{CH}_3(\text{CH}_2)_3\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}_3$	RL	298	$\geq 3.3(-1)$			2/2
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$ (a) $\rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ (b)						
Methyl + Butyl, 1-methyl-						
71 WAT $(k_a + k_b)/k_a$.	RL	298	1.16			2/2
$\text{CH}_3 + (\text{CH}_3)_4\text{C} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CCH}_2$						
Methyl + Propane, 2,2-dimethyl- (Neopentane)						
71 MCN/KEL k_{ref} : $\text{CH}_3 + \text{CD}_2=\text{C}=\text{O} \rightarrow \text{CH}_3\text{D} + \text{CD}=\text{C}=\text{O}$	RL	653	(6.7 ± 0.9)			2/2
73 PAC	RN	793-953	3.16(13)	0	8059 $\pm$ 241	2 1.26
76 BRA/WES1 Computer data-fit to a proposed mechanism.	DE	1030-1300	6.6(14)	0	10826	2 1.66
72 FUR/LAI2 Hg-photosensitized decomposition of Neopentane. k determined relative to the reaction: $\text{CH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_3$	RN	529-608	4.9(11)	0	5788	2
78 MAR/COM Stirred flow-reactor pyrolysis. $P(\text{Neopentane}) = 50$ torr.	EX	703-743	5.01(11)	0	5184	2
78 PAC/WIM Neopentane flow-pyrolysis. $P = 7.6$ torr.	EX	821	$(1.36 \pm 0.16)(9)$			2
80 PAC/WIM1 Pyrolysis of Neopentane in a flow-reactor. Gas-chromatography. $P = (4-335)$ torr.	EX	823	$(1.6 \pm 0.1)(9)$			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3 + \text{CH}_3\text{C}(\text{O})\text{C}(\text{O})\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_2\text{C}(\text{O})\text{C}(\text{O})\text{CH}_2\text{CH}_3$ (a)						
$\rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{O})\text{C}(\text{O})\text{CHCH}_3$ (b)						
$\rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{O})\text{C}(\text{O})\text{CH}_2\text{CH}_2$ (c)						
$\rightarrow (\text{CH}_3)_2\text{CO} + \text{CH}_3\text{CH}_2\text{CO}$ (d)						
Methyl + 2,3-Pentanedione						
74 SCH/KNO k_b/k_a . T-dependence not detectable.	RL	362-398	≈ 4.5	0	0	2/2
74 SCH/KNO k_c/k_a . T-dependence not detectable.	RL	362-398	$\approx 3.0(-1)$	0	0	2/2
74 SCH/KNO $(k_a + k_b + k_c)/k_d$.	RL	362-398	2.51(1)	0	151±654	2/2 2.51
$\text{CH}_3 + \text{CH}_3\text{CD}_2\text{C}(\text{O})\text{CD}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_2\text{CD}_2\text{C}(\text{O})\text{CD}_2\text{CH}_3$ (a)						
$\rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{CDC}(\text{O})\text{CD}_2\text{CH}_3$ (b)						
Methyl + 3-Pentanone-2,2,4,4-d ₄						
72 SCH/WOL1 k_a .	EX	513-572	2.00(11)	0	5544±454	2 3.16
72 SCH/WOL1 k_b .	EX	513-572	1.26(11)	0	4177±201	2 1.78
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3$ (a)						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)_2\text{CH}_2$ (b)						
$\rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CHC}(\text{CH}_3)=\text{CH}_2$ (c)						
$\rightarrow \text{CH}_4 + \text{CH}_2\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ (d)						
$\rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(=\text{CH}_2)\text{CH}_2$ (e)						
Methyl + 1-Pentene, 2-methyl-						
74 SHI/AMA k_a/k_b .	RL	923	5.0			2/2
74 SHI/AMA $(k_a + k_b)/(k_c + k_d + k_e)$.	RL	923	6.0(-1)			2/2
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}=\text{C}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{C}(\text{CH}_3)_2$ (a)						
$\rightarrow \text{CH}_3\text{CH}_2\text{CHC}(\text{CH}_3)_3$ (b)						
$\rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}=\text{C}(\text{CH}_3)\text{CH}_2$ (c)						
$\rightarrow \text{CH}_4 + \text{CH}_3\text{CHCH}=\text{C}(\text{CH}_3)_2$ (d)						
Methyl + 2-Pentene, 2-methyl-						
74 SHI/AMA k_a/k_b .	RL	923	1.0			2/2
74 SHI/AMA $(k_a + k_b)/(k_c + k_d)$.	RL	923	1.2(-1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3 + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3(\text{CH}_2)_4\text{CH}_2$ (a) $\rightarrow \text{CH}_4 + \text{CH}_3(\text{CH}_2)_3\text{CHCH}_3$ (b) $\rightarrow \text{CH}_4 + \text{CH}_3(\text{CH}_2)_2\text{CHCH}_2\text{CH}_3$ (c)						
Methyl + Hexane						
76 YAM $k_a + k_b + k_c$.	RN	973-1088	4.2(12)	0	5637	2
$\text{CH}_3 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}_2$ (a) $\rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CCH}(\text{CH}_3)_2$ (b)						
Methyl + Butane, 2,3-dimethyl-						
75 BUL/MAR ¹⁾ k_b/k_a . Estimated ratio.	RL	667-770	1.0(-1)	0	-2526	2/2
75 BUL/MAR ¹⁾ $k_a + k_b$.	ES	667-770	2.00(13)	0	7217	2
¹⁾ Static system pyrolysis.						
$\text{CH}_3 + \text{CH}_3\text{C}(\text{O})\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3$ $\rightarrow \text{CH}_4 + \text{CH}_2\text{C}(\text{O})\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3$ (a) $\rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{O})\text{CHCH}_2\text{C}(\text{O})\text{CH}_3$ (b) $\rightarrow (\text{CH}_3)_2\text{CO} + \text{CH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3$ (c)						
Methyl + 2,5-Hexanedione						
75 KNO/SCH $(k_a + k_b)/k_c$.	RL	515-712	1.0	0	-1631±10	2/2
75 KNO/SCH $k_a + k_b$.	CO	515-712	3.16(11)	0	4026	2
75 KNO/SCH k_c .	RN	515-712	3.16(11)	0	5637	2
$\text{CH}_3 + (\text{CH}_3)_3\text{COOC}(\text{CH}_3)_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{COOC}(\text{CH}_3)_2\text{CH}_2$						
Methyl + Peroxide, bis(1,1-dimethylethyl)-						
80 KNO/RIC ¹⁾ k_{ref} :	RL	413	(3.5±0.3)			2/2
$\text{CH}_3 + (\text{CD}_3)_2\text{CO} \rightarrow \text{CH}_3\text{D} + \text{CD}_2\text{C}(\text{O})\text{CD}_3$						
80 KNO/RIC ¹⁾	RN	413	(1.06±0.12)(6)			2
¹⁾ Thermolysis of Azomethane and di-t-Butylperoxide. Mass-spectrometry.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₄ (+ M) → CH₃ + H (+ M) (a)						
→ any other products (b)						
Methane						
71 DEA/KIS k _a . M = Ar. Shock-waves. Best-fit to experimental data. Total conc.: 5x10 ¹⁷ molec.cm ⁻³ .	DE	1750-2575	1.63(18)	0	51837	2
71 HAR/TRO k _a . M = Ar. Limiting high-pressure k.	EX	1850-2500	1.26(15)	0	52340±1007	1
71 HAR/TRO k _a . M = Ar. Low-pressure k.	EX	1850-2500	2.00(17)	0	44288±1007	2
72 NAP/SUB k _a . M = Ar.	EX	1750-2700	3.8(13)	0	47106	1
73 VOM2 k _a . M = Ne. The experimental conditions correspond to the limiting case of low pressures.	EX	2000-2700	3.98(9)	0	31706±2516	1 3.16
75 BOW1 k _a . M = Ar.	ES	1900-2400	1.4(17)	0	44500	2
75 CHE/BAC k _a . Limiting high-pressure k.	EX	995-1103	2.8(16)	0	54152	1
75 GAR/OWE k _a . M = H ₂ , Ne, Ar, Kr.	EX	2000-2700	2.3(14)	0	32477	2
75 ROT/JUS k _a . M = Ar.	EX	1700-2300	4.73(17)	0	46911	2
77 HEF/PAR k _a . M = Ar.	EX	2023-2721	2.2(17)	0	45345	2
78 FEN/SUL k _a . M = Ar. CH ₄ pyrolysis in reflected shock-waves. He/Ne Laser-absorption. P(Total) = (2.3-4.2) atm.	EX	2023-2721	2.2(17)	0	45345	2
79 TAB/BAU k _a . M = Ar. CH ₄ pyrolysis behind shock-waves. Total conc.: (1.4-5.4)x10 ¹⁸ molec.cm ⁻³ .	EX	1950-2770	(1.01±0.23)(17)	0	43181±503	2
80 ROT k _a . M = Ar. CH ₄ Thermolysis behind shock-waves. Atomic Resonance-Absorption Spectrophotometry. Same data published in 79 ROT/JUS1.	EX	1800-2300	4.73(17)	0	46800	2
82 KLO/DRO k _{overall} . M = Ar. CH ₄ pyrolysis behind single-pulse shock-waves. High-pressure. P = (6-10) atm.	EX	1500-3000	1.0(15)	0	51482	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CD₄ (+ M) → CD₃ + D (+ M)						
Methane-d ₄						
80 CHI/BAK ¹⁾	EX	1780-2440	1.4(11)	0	40765	1
80 CHI/BAK ¹⁾	EX	1780-2440	2.1(16)	0	42728	2
M = Ar.						
¹⁾ CD ₄ Pyrolysis behind shock-waves. Resonance-Absorption Spectroscopy.						
CHO (+ M) → CO + H (+ M)						
Methyl, oxo- (Formyl)						
76 TSU	DE	1500-2000	1.0(14)	0	11066	2
M = r. Computer calculation on the basis of a suggested mechanism.						
CHO + O₂ (+ M) → CO + HO₂ (+ M) (a)						
→ CO ₂ + OH (+ M) (b)						
→ HCO ₃ (+ M) (c)						
Methyl, oxo- (Formyl) + Oxygen molecule						
74 WAS/MAR	RL	297	(2.74±0.21)(-2)			2/2
k _a /k _{ref} . k _{ref} : O + CHO → H + CO ₂ (d) → OH + CO (e)						
81 MOR/HEI	RL	296	(2.1±0.7)(-1)			2/2
k _a /k _{ref} . Photolysis of NO ₂ in presence of HCHO and O ₂ , at 360 nm. P(Total) = 52 torr. k _{ref} : NO ₂ + CHO → NO + HCOO						
73 PEE/MAH1	ES	1600	≈3.0(13)			2
k _a . Tentative k.						
74 WAS/MAR	RN	297	(3.43±0.72)(12)			2
k _a . Ethylene used as source of CHO.						
76 MAR	RN	297	(4.70±2.59)(12)			2
k _a . Formaldehyde used as source of CHO.						
77 SHI/EBA	EX	298	(5.12±0.60)(12)			2
k _a .						
78 CLA/MOO	EX	298	(2.41±0.48)(12)			2
k _a . Monochromatic laser photolysis.						
78 REI/CLA	EX	298	(2.41±0.48)(12)			2
k _a . HCHO photolysis with tunable pulsed UV-laser.						
81 CHE/RHO	DE	250-2000	(3.5±0.5)(12)	0	0	2
k _a . Kinetic modelling Of CO oxidation in flames.						
81 GIL/JOH	EX	298	(2.53±0.42)(12)			2
k _a . CH ₃ CHO Flash-photolysis. Time-resolved intracavity laser detection. P(CH ₃ CHO) = 0.2 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 VEY/LES k _a . CHO generated by Flash-photolysis of HCHO, or CH ₃ CHO. Laser-Resonance-absorption. The pre- exponential factor expressed as: A(T/298) ^{-0.4} . P(Total) = 45, or 500 torr.	EX	298-503	3.39(12)	-0.4	0	2
76 OSI/HEI k _b /k _a . Upper-limit ratio.	RL	296	≤1.9(-1)			2/2
79 NAD/SAR3 ¹⁾ k _b /k _a . Flash-photolysis of CH ₃ CHO, or HCHO. P(Total) = (13-100) torr.	RL	298	1.9(-1)			2/2
76 OSI/HEI k _c /k _{ref} . k _{ref} : CHO + O ₂ → CO + HO ₂	RL	296	(5.0±1.0)			2/2
79 NAD/SAR3 ¹⁾ k _c /k _a . Flash-photolysis of CH ₃ CHO, or HCHO. P(Total) = (13-100) torr.	RL	298	(5.0±1.0)			2/2
79 NAD/SAR3 ¹⁾ k _a + k _b + k _c . CH ₃ CHO flash-photolysis.	EX	298	(2.41±0.60)(12)			2
79 NAD/SAR3 ¹⁾ k _a + k _b + k _c . HCHO flash-photolysis. ¹⁾ Intracavity laser spectroscopy. P(Total) = (3-100) torr.	EX	298	(2.23±0.48)(12)			2
78 HOR/SU k _c . HCHO photolysis at 313 nm. Lower-limit k. P(HCHO) = 8 torr. P(CO ₂) = (0-300) torr. P(O ₂) = (0.02-8) torr.	EX	298	≥(4.4±1.6)(17)			3
CHO + NO → CO + HNO						
Methyl, oxo- (Formyl) + Nitrogen oxide (NO)						
77 SHI/EBA	EX	298	(3.37±0.54)(12)			2
78 CLA/MOO Monochromatic laser photolysis.	EX	298	(8.73±1.20)(12)			2
78 REI/CLA HCHO photolysis with tunable pulsed UV-laser.	EX	298	(8.43±1.20)(12)			2
80 NAD/SAR CH ₃ CHO/HCHO/NO Flash-photolysis. Pulse-photolysis. Intracavity laser spectroscopy. P(Total) = (13-100) torr.	EX	298	(7.22±2.41)(12)			2
81 VEY/LES CHO generated by Flash-photolysis of HCHO, or CH ₃ CHO. Laser Resonance-absorption. P(Total) = 45, or 500 torr. The preexponential factor expressed as: A(T/298) ^{-0.4} .	EX	298-503	7.40(12)	-0.4	0	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CHO + NO₂ → HCOO + NO						
Methyl, oxo- (Formyl) + Nitrogen oxide (NO ₂)						
80 MOR/HEI NO ₂ /HCHO Photolysis at 366 nm. IR-Absorption spectroscopy. k _{ref} : NO ₂ + CHO → HCOONO (a) → HCONO ₂ (b)	RL	296	≈(1.07±0.13)			2/2
81 MOR/HEI ¹⁾ k _{ref} : O ₂ + CHO → HO ₂ + CO.	RL	296	(2.1±0.7)(-1)			2/2
81 MOR/HEI ¹⁾ ¹⁾ NO ₂ /HCHO/O ₂ Photolysis at 360 nm. P(Total) = 52 torr.	RN	296	(1.63±0.54)(13)			2
CHO + CHO → CO + CO + H₂ (a) → HCHO + CO (b) → OHCCCHO (c)						
Methyl, oxo- (Formyl)						
79 FOE/BER k _a /k _c . Butanal photolysis. Rate ratio derived from a suggested reaction scheme.	RL	253-298	(8.0±2.0)	0	0	2/2
78 HOR/CAL k _b /k _a . HCHO Photolysis at 313 nm. P(HCHO) = (1-12) torr.	EX	298	5.8			2
78 REI/CLA k _b . HCHO photolysis with tunable pulsed UV-laser. Preliminary k.	EX	298	3.80(13)			2 3.2
79 FOE/BER k _b /k _c . Butanal photolysis. Rate ratio derived from a suggested reaction scheme.	RL	253-298	(1.7±0.5)	0	0	2/2
79 NAD/SAR2 k _a + k _b + k _c . Pulse-photolysis of CH ₃ CHO. Gas-chromatography.	EX	298	(1.81±0.72)(13)			2
79 NAD/SAR4 k _a + k _b + k _c . Intracavity laser spectroscopy. Unreported T assumed to be 298 K. Lower-limit k.	EX	298	>3.0(12)			2
80 HOC/SWO1 k _a + k _b + k _c . H ₂ flash-photolysis in presence of CO. P = 760 torr.	EX	298	(1.4±0.3)(13)			2
80 MUL k _a + k _b + k _c . CH ₃ CHO decomposition by pulsed UV-Photolysis. Internal resonator Laser-Spectroscopy.	EX	298	(2.15±0.34)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CHO + CH₃CH₂CH₂ → CO + CH₃CH₂CH₃							
Methyl, oxo- (Formyl) + Propyl							
79 FOE/BER Butanal photolysis. k derived from a suggested reaction scheme.	DE	253-298	3.16(13)	0	0	2	1.58
CHO + CH₃CH₂CH₂CHOH → CO + CH₃CH₂CH₂CH₂OH							
Methyl, oxo- (Formyl) + Butyl, 1-hydroxy-							
79 FOE/BER Butanal photolysis. T-independent. Derived from a suggested reaction scheme. k _{ref} : CH ₃ CH ₂ CH ₂ + CH ₃ CH ₂ CH ₂ CHOH → (CH ₃ CH ₂ CH ₂) ₂ CHOH	RL	253-298	(4.1±1.4)	0	0	2/2	
HCHO* (or HC(:)OH) → H + CHO (a)							
→ H ₂ + CO (b)							
Formaldehyde (or Methylene, hydroxy-)							
79 MOR/HEI k _a /(k _a + k _b). HCHO photolysis at 313 nm.	RL	296	(6.1±1.5)(-1)			1/1	
HCHO (+ M) → H + CHO (+ M) (a)							
→ H ₂ + CO (+ M) (b)							
Formaldehyde							
81 TSU/KAT ¹⁾ Total conc. = 6.0x10 ¹⁸ molec.cm ⁻³ .	ES	1500-1900	6.92(11)	0	36206	1	
81 TSU/KAT ¹⁾ Total conc. = 3.0x10 ¹⁹ molec.cm ⁻³ .	ES	1500-1900	2.51(12)	0	36206	1	
81 TSU/KAT ¹⁾ Total conc. = 6.0x10 ¹⁹ molec.cm ⁻³ .	ES	1500-1900	3.55(12)	0	36206	1	
¹⁾ k _a . M = Ar. CH ₃ OH/O ₂ thermal oxidation. Reflected shock-waves. UV-absorption.							
75 BOW1 k _a . M = Ar.	ES	1900-2400	1.0(14)	0	18500	2	
79 DEA/CRA k _a . M = Ar. Reflected shock waves. [HCHO] = (2.4-4.5)x10 ¹⁸ molec.cm ⁻³	EX	1800-2500	3.61(17)	0	43784±6014	2	2.95
80 DEA/JOH1 k _a . M = Ar. HCHO Decomposition behind shock-waves. Best data-fit. Total conc. = 5x10 ¹⁸ molec.cm ⁻³ .	EX	1700-2500	3.31(16)	0	40777	2	
73 PEE/MAH1 k _b . M = O ₂ , H ₂ O, CO ₂ .	EX	1100-1900	2.1(16)	0	17614±2516	2	
77 MIY/MOR k _b . Calculation based on a proposed mechanism.	DE	500-2090	2.1(15)	0	17620	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 VAN/VAN k_b . M = Ar. $\text{CH}_3\text{OH}/\text{O}_2$ lean flames at 40 torr. Molecular beam sampling. Mass-spectrometry.	DE	1000-2000	2.5(14)	0	14595	2	
82 KLI/PEN k_b . M = H_2 . HCHO/Ar Pyrolysis behind reflected shock-waves. P = (1.8-2.7) torr.	EX	1200-2200	2.4(13)	0	8254	2	
DCDO (+ M) $\rightarrow$ D + D + CO (+ M)							
Formaldehyde- d_2							
80 CHI/SKI M = Ar. $\text{CD}_4/\text{O}_2/\text{Ar}$ oxidation behind reflected shock-waves. Resonance-Absorption.	EX	1700-2200	4.5(16)	0	36206	2	
$\text{HCOOH} (+ \text{M}) \rightarrow \text{CO} + \text{H}_2\text{O} (+ \text{M})$ (a) $\rightarrow \text{CO}_2 + \text{H}_2 (+ \text{M})$ (b)							
Formic acid							
71 BLA/DAV ¹⁾ k_a .	EX	943-1053	2.45(12)	0	30432	1	
71 BLA/DAV ¹⁾ k_b . Static vessel.	EX	730-1053	2.95(9)	0	24417 $\pm$ 854	1	2.95
71 BLA/DAV ¹⁾ k_b . Unpacked flow vessel.	EX	730-1053	2.75(8)	0	22962 $\pm$ 349	1	1.48
71 BLA/DAV ¹⁾ k_b . Packed flow-vessel.	EX	730-1053	3.98(9)	0	26523 $\pm$ 445	1	1.59
¹⁾ HCOOH Pyrolysis. Flow, or static system. P = (20-230) torr.							
76 SAM/PET ²⁾ Based on $E_a(\text{CHClF}_2) = (55.0 \pm 2.5) \text{ kcal.mol}^{-1}$.	EX	900-1000	3.16(14)	0	33216 $\pm$ 1912	1	7.94
76 SAM/PET ²⁾ Based on $E_a(\text{CHClF}_2) = (55.8 \pm 2.5) \text{ kcal.mol}^{-1}$.	EX	900-1000	1.0(15)	0	33568 $\pm$ 2013	1	7.94
76 SAM/PET ²⁾ Based on $E_a(\text{CHClF}_2) = (51.4 \pm 2.5) \text{ kcal.mol}^{-1}$.	EX	900-1000	3.16(13)	0	31052 $\pm$ 1812	1	6.31
²⁾ $k_a + k_b$. Chanel (a) is predominant. $\text{HCOOH}/\text{CHClF}_2$ Decomposition induced by a CO_2 laser. P(HCOOH) = 1.5 torr. P(CHClF_2) = 4 torr.							
82 HSU/SHA ³⁾ k_a . M = Ar.	EX	1280-2030	2.3(15)	0	25164 $\pm$ 856	2	
82 HSU/SHA ³⁾ k_b .	EX	1280-2030	1.5(16)	0	28686 $\pm$ 1409	2	
³⁾ M = Ar. HCOOH Pyrolysis behind incident, or reflected shock-waves. Laser-probing apparatus. P(Total) = (0.75-2.8) atm. [HCOOH] = (0.07-1.6)%							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
HCOOH + HCOOH → HCHO + CO₂ + H₂O						
Formic acid						
71 BLA/DAV HCOOH pyrolysis in a flow, or static system. Gas-chromatography. Above 873 K the Arrhenius plot becomes curved but straightens out again above 943 K, to become first order. P = (20-230) torr.	EX	730-873	2.75(11)	0	15938	2
CH₃O (+ M) → HCHO + H (+ M) (a) → CH₂OH (+ M) (b)						
Methoxy						
79 BAT k _a . Conventional static system.	ES	393-473	1.58(14)	0	13840±503	1 3.16
81 BAT/BUR k _b . Probably an upper-limit k.	ES	393-473	1.0(13)	0	13078±1151	1 3.16
82 GUT/SAN k _b . CH ₃ ONO photolysis at 266 nm. Laser-induced fluorescence. M = N ₂ , or SF ₆ . P-independent. Upper-limit k. P = (10-100) torr.	ES	298	<2.0(2)			1
CH₃O* → HCHO + H						
Methoxy						
73 WIE/HEI M = N ₂ . k _{ref} : CH ₃ O* + M → CH ₃ O + M. CH ₃ O* formed by photolysis of CH ₃ ONO at 366 nm.	RL	298	1.04(-7)			1/2
CH₃O + O₂ → HCHO + HO₂						
Methoxy + Oxygen molecule						
73 WIE/VIL k _{ref} : CH ₃ O + NO → HCHO + HNO + CH ₃ ONO	RL	298	4.7(-5)			2/2
75 ALC/MIL	ES	373	1.2(9)			2
75 GLA k _{ref} : CH ₃ O + NO → CH ₃ ONO	RL	296	(5.2±0.7)(-5)			2/2
75 GLA Upper-limit ratio. k _{ref} : CH ₃ O + NO ₂ → CH ₃ ONO ₂	RL	296	≤(7.4±0.7)(-5)			2/2
75 MEN/GOL	ES	300	3.5(8)			2
77 ALC/MIL ¹⁾ Estimated ratio. k _{ref} : CH ₃ + (CH ₃) ₂ CHCH(CH ₃) ₂ → CH ₃ OH + (CH ₃) ₂ CHC(CH ₃) ₂	RL	373	(5.8±0.8)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k _A units	k err. factor
77 ALC/MIL ¹) Estimated ratio. k _{ref} : $\text{CH}_3\text{O}_2 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{OOH} + (\text{CH}_3)_2\text{CHC}(\text{CH}_3)_2$	RL	373	3.3			2/2	
77 ALC/MIL ¹) ¹) Azomethane photolysis.	ES	373	1.2(9)			2	
77 BAR/BEN1 Vacuum technique. Chromatography.	RN	396-442	3.16(11)	0	2013±1409	2	31.6
79 BAT/RAT Static system. Gas-chromatography.	EX	383-433	1.0(12)	0	2265±554	2	4.0
79 BAT/ROB Static system. Gas-chromatography.	EX	383-433	1.0(12)	0	2416±554	2	4.0
80 COX/DER2 ONOC ₃ photolysis. Gas-chromatography.	EX	296-450	7.59(10)	0	1352±340	2	2.5
80 SAN/BUT2 CH ₃ ONO photolysis at 266 nm. Laser-induced Fluorescence. Upper-limit k. P (Max) = 50 torr. Same data published in 80 SAN/BUT1.	EX	298	<1.20(9)			2	
81 KIR/PAR Azo-t-butane/O ₂ photolysis. Upper-limit ratio. k _{ref} : $\text{CH}_3\text{O} + (\text{CH}_3)_3\text{COOH} \rightarrow \text{CH}_3\text{OH} + (\text{CH}_3)_3\text{CO}_2$	RL	373	<4.0(-1)			2/2	
82 GUT/SAN CH ₃ ONO photolysis at 266 nm. Laser-induced fluorescence. P(O ₂ + N ₂) = 40 torr.	EX	413-628	6.3(10)	0	1309	2	
CH₃O + O₃ → products							
Methoxy + Ozone							
75 SIM/HEI Upper-limit k.	EX	298	<1.20(9)			2	
CH₃O + NO → HCHO + HNO (a)							
→ CH₃ONO (b)							
Methoxy + Nitrogen oxide (NO)							
73 WIE/HEI ¹) Electronically excited ONOC ₃ .	RL	298-423	1.45(-1)	0	0	2/2	
73 WIE/VIL ¹)	RL	298	1.45(-1)			2/2	
75 GLA ¹) ¹) k _a /(k _a + k _b).	RL	296	1.3(-1)			2/2	
75 BAT/MCC ²)	ES	393-473	3.98(12)	0	0±503	2	3.16
77 BAT/MIL3 ²) ²) k _a .	ES	440-473	2.0(12)	0	0±503	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
73 WIE/VIL ($k_a + k_b$)/ k_{ref} . k_{ref} : $CH_3O + NO_2 \rightarrow HCHO + HONO$ (c) $\rightarrow CH_3ONO_2$ (d)	RL	298	1.2				2/2
80 SAN/BUT2 $k_a + k_b$. M = SF_6 . CH_3ONO photolysis at 266 nm. Laser-induced fluorescence. Limiting high-pressure k. Same data given in 80 SAN/BUT1.	EX	298	(1.3±0.1)(13)				2
79 BAT/RAT k_b/k_{ref} . Static system. Spherical and packed reaction vessels. CH_3O generated by CH_3OOCH_3 decomposition. k_{ref} : $CH_3O + NO_2 \rightarrow CH_3ONO_2$. [NO_2] = (3.73-4.10)×10 ¹⁶ molec.cm ⁻³ . [NO] = (2.65-2.77)×10 ¹⁷ molec.cm ⁻³ . [CH_3OOCH_3] = 6.0×10 ¹⁶ molec.cm ⁻³ .	RL	420	(2.03±0.47)				2/2
74 BAT/MIL ³⁾	ES	393-473	1.26(13)	0	0±503	2	2.51
75 BAT/MCC ³⁾	ES	393-473	1.26(13)	0	0±503	2	2.51
77 BAT/MIL3 ³⁾	ES	440-473	1.26(13)	0	0±503	2	3.98
³⁾ k_b .							
$CH_3O + NO_2 \rightarrow HCHO + HONO$ (a) $\rightarrow CH_3ONO_2$ (b)							
Methoxy + Nitrogen oxide (NO_2)							
77 BAR/BEN1 ¹⁾ k_a/k_b . Assumed to be T-independent.	RL	396-442	(3.0±0.5)(-1)	0	0	2/2	
77 BAR/BEN1 ¹⁾ k_a .	RN	396-442	2.0(9)	0	0	2	
¹⁾ Vacuum technique. Chromatography.							
77 BAT/MIL3 k_a .	ES	440-473	5.01(11)	0	0	2	
73 WIE/VIL $k_b/(k_a + k_b)$.	RL	298	9.2(-1)				2/2
77 BAR/BEN1 k_b . Review of literature data.	SE	396-442	6.31(12)	0	0	2	3.16
77 BAT/MIL3 k_b .	ES	440-473	5.01(12)	0	0	2	
79 BAT/RAT k_b . Static system. Spherical and packed reaction vessels. CH_3O generated by CH_3OOCH_3 decomposition. [CH_3OOCH_3] = 6.0×10 ¹⁶ molec.cm ⁻³ . [NO_2] = (3.73-4.10)×10 ¹⁶ molec.cm ⁻³ . [NO] = (2.65-2.77)×10 ¹⁷ molec.cm ⁻³ .	RN	420	7.94(12)			2	2.51

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃O + N₂O → products							
Methoxy + Nitrogen oxide (N ₂ O)							
80 SAN/BUT2 CH ₃ ONO photolysis at 266 nm. Laser-induced fluorescence. P(Max) = 5 torr. Upper-limit k.	EX	298	<1.20(10)			2	
CH₃O + NH₃ → CH₃OH + NH₂							
Methoxy + Ammonia							
80 SAN/BUT2 CH ₃ ONO photolysis at 266 nm. Laser-induced fluorescence. P(Max) = 1 torr. Upper-limit k.	EX	298	<6.02(10)			2	
CH₃O + CO → CH₃ + CO₂ (a)							
→ any other products (b)							
Methoxy + Carbon monoxide							
73 LIS/MAS k _a .	EX	396-426	1.6(13)	0	5939±755	2	3.98
73 WIE/HEI k _{overall} /k _{ref} . Assumed to be T-independent. k _{ref} : CH ₃ O + NO → HCHO + HNO (c) → CH ₃ ONO* (d)	RL	298-423	~5.0(-4)	0	0	2/2	
80 SAN/BUT2 k _{overall} . CH ₃ ONO photolysis at 266 nm. Laser-induced fluorescence. Upper-limit k. P(Max) = 10 torr.	EX	298	<6.02(9)			2	
CH₃O + CH₄ → products							
Methoxy + Methane							
80 SAN/BUT2 CH ₃ ONO photolysis at 266 nm. Laser-induced fluorescence. P(Max) = 10 torr. Upper-limit k.	EX	298	<6.02(9)			2	
CH₃O + CH₃O → HCHO + CH₃OH (a)							
→ CH ₃ OOCH ₃ (b)							
Methoxy							
73 SHO/HEI k _a /k _b .	RL	298	8.9			2/2	1.3
75 WEA/SHO ¹⁾ k _a /(k _a + k _b).	RL	288	1.0			2/2	
79 HAS/KOS k _a . Flash-photolysis of CH ₃ COOCH ₃ . Gas-chromatography. P = (1.5-700) torr.	EX	298	2.32(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 BAT/MCC1 k_b .	ES	383-413	2.0(13)	0	0	2 3.16
75 WEA/SHO ¹⁾ $k_b/(k_a + k_b)$.	RL	288	~0			2/2
¹⁾ Azomethane Photolysis.						
77 BAR/BEN2 k_b . VLP-Pyrolysis. RRKM best-fit estimate.	ES	391-432	5.01(12)	0	0	2
CD₃O + CD₃O → DCDO + CD₃OD (a)						
→ CD₃OCD₃ (b)						
Methoxy-d ₃						
75 WEA/SHO ¹⁾ $k_a/(k_a + k_b)$.	RL	288	1.0			2/2
75 WEA/SHO ¹⁾ $k_b/(k_a + k_b)$.	RL	288	~0			2/2
¹⁾ Azomethane-d ₆ Photolysis.						
CH₃O + CH₃OH → products						
Methoxy + Methanol						
80 SAN/BUT2 CH ₃ ONO photolysis at 266 nm. Laser-induced fluorescence. Upper-limit k. P(Max) = 1 torr. Same data given in SAN/BUT1.	EX	298	<6.02(10)			2
CH₃O + CH₂=CH₂ → CH₃OCH₂CH₂						
Methoxy + Ethene						
75 LIS/MAS	RN	300	(3.7±0.8)(7)			2
CH₃O + CH₃CO → HCHO + CH₃CHO						
Methoxy + Ethyl, 1-oxo- (Acetyl)						
79 HAS/KOS CH ₃ C(O)OCH ₃ Flash-photolysis. P = (1.5-700) torr.	EX	298	3.42(13)			2
CH₃O + CH₃CHO → CH₃OH + CH₃CO						
Methoxy + Acetaldehyde						
75 WEA/MEA Estimated ratio. k_{ref} : CH ₃ O + O ₂ → HCHO + HO ₂	RL	298	~(1.5±0.5)(1)			2/2
75 WEA/MEA	ES	298	(2.55±0.85)(9)			2
78 KEL/HEI ¹⁾ k_{ref} : CH ₃ O + O ₂ → HCHO + HO ₂	RL	298	(1.40±0.28)(1)			2/2
78 KEL/HEI ¹⁾ ¹⁾ Azomethane photolysis.	RN	298	(5.0±1.0)(9)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$\text{CH}_3\text{O} + \text{CH}_3\text{OOCH}_3 \rightarrow \text{CH}_3\text{OH} + \text{HCHO} + \text{CH}_3\text{O}$							
Methoxy + Peroxide, dimethyl-							
77 BAR/BEN1 Vacuum technique. Chromatography.	ES	391-432	$\approx 5.0(7)$	0	0	2	
$\text{CH}_3\text{O} + (\text{CH}_3)_3\text{C} \rightarrow (\text{CH}_3)_3\text{COCH}_3$							
Methoxy + Ethyl, 1,1-dimethyl- (t-Butyl)							
76 BAT/MCC1	ES	383-413	5.01(12)	0	0	2	
$\text{CH}_3\text{O} + (\text{CH}_3)_3\text{CH} \rightarrow \text{CH}_3\text{OH} + (\text{CH}_3)_3\text{C}$							
Methoxy + Propane, 2-methyl-							
79 BAT/RAT Static system.	EX	383-433	3.98(11)	0	1208 $\pm$ 554	2	3.98
80 SAN/BUT2 CH_3ONO photolysis at 266 nm. Laser-induced Fluorescence. Upper-limit k. P(Max) = 0.5 torr. Same data given in 80 SAN/BUT1.	EX	298	<1.20(11)			2	
$\text{CH}_3\text{O} + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{products}$							
Methoxy + 1-Butene							
80 SAN/BUT2 CH_3ONO photolysis at 266 nm. Laser-induced Fluorescence. Upper-limit k. P(Max) = 0.25 torr. Same data given in 80 SAN/BUT1.	EX	298	<2.41(11)			2	
$\text{CH}_3\text{O} + (\text{CH}_3)_3\text{COOH} \rightarrow \text{CH}_3\text{OH} + (\text{CH}_3)_3\text{CO}_2$							
Methoxy + Hydroperoxide, 1,1-dimethylethyl- (t-Butyl hydroperoxide)							
81 KIR/PAR Azo-t-butane/ O_2 Photolysis. Lower-limit k, determined relative to reaction: $\text{CH}_3\text{O} + \text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2$	RN	373	>4.22(9)			2	
$\text{CH}_3\text{O} + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{OH} + (\text{CH}_3)_2\text{CHC}(\text{CH}_3)_2$							
Methoxy + Butane, 2,3-dimethyl-							
75 ALC/MIL	ES	373	4.0(8)			2	
$\text{CH}_2\text{OH} (+\text{M}) \rightarrow \text{HCHO} + \text{H} (+\text{M})$							
Methyl, hydroxy-							
75 BOW2 M = Ar. Reflected shock waves. Best data-fit. [Ar] = (5.7-17.0) $\times 10^{18}$ molec.cm ⁻³ . [CH ₂ OH] = 1.3 $\times 10^{17}$ molec.cm ⁻³ .	ES	1545-2180	3.0(9)	0	14600	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 TSU/KAT ¹⁾ Total conc. = 6.0×10^{18} molec.cm ⁻³ .	CO	1500-1900	1.3(10)	0	14550	1
81 TSU/KAT ¹⁾ Total conc. = 3.0×10^{19} molec.cm ⁻³ .	CO	1500-1900	5.6(10)	0	14550	1
81 TSU/KAT ¹⁾ Total conc. = 6.0×10^{19} molec.cm ⁻³ .	CO	1500-1900	1.0(11)	0	14550	1
¹⁾ M = Ar. CH ₃ OH/O ₂ thermal oxidation in Ar, behind reflected shock-waves. Same data given in 81 TSU/HAS.						
CH₂OH + O₂ → HCHO + HO₂						
Methyl, hydroxy- + Oxygen molecule						
80 RAD M = He. Flow-tube. LMR-spectroscopy. P(He) = 0.5 torr.	EX	300	1.20(12)			2 2.0
81 TSU/HAS M = Ar. CH ₃ OH/O ₂ thermal oxidation behind reflected shock-waves.	ES	1200-1800	1.0(13)	0	0	2
81 VAN/VAN CH ₃ /O ₂ oxidation in lean flames. Molecular beam sampling. Mass-spectrometry. P = 40 torr.	DE	1000-2000	1.0(14)	0	2516	2
CH₂OH + H₂O → CH₃OH + OH						
Methyl, hydroxy- + Water						
81 TSU/HAS M = Ar.	CO	1200-1800	1.55(14)	0	13231	2
CH₂OH + H₂O₂ → CH₃OH + HO₂						
Methyl, hydroxy- + Hydrogen peroxide						
81 TSU/HAS M = Ar.	CO	1200-1800	2.69(11)	0	-241	2
CH₃O₂ + O₃ → products						
Methyldioxy + Ozone						
75 SIM/HEI Upper-limit k.	EX	298	<1.45(7)			2
CH₃O₂ + SO₂ → CH₃O + SO₃ (a) → CH₃O₂SO₂ (b)						
Methyldioxy + Sulfur dioxide						
78 WHI/BOT k _a . Kinetic spectroscopy. Upper-limit k.	EX	298	≤2.0(9)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 SIM/HEI k_b/k_{ref} . Azomethane/ O_2 / SO_2 /NO photolysis. k_{ref} : $CH_3O_2 + NO \rightarrow CH_3O + NO_2$.	RL	296	(2.5±0.5)(-3)			2/2
81 KAN/CAL k_b . Azomethane/ SO_2 /Air photolysis. FTIR-Spectroscopy. $P(O_2) = 100$ torr. $P(N_2) = 600$ torr.	EX	298	(8.43±1.20)(9)			2
79 KAN/MCQ ¹⁾	ES	298	≤(3.2±0.7)(9)			2
79 KAN/MCQ ¹⁾	ES	298	≤(6.4±1.4)(9)			2
¹⁾ $k_a + k_b$. Azomethane/Oxygen Flash-photolysis. k estimated as 1/2 of the measured apparent k. The lower limit estimate probably most nearly correct.						
79 SAN/SIM $k_a + k_b$. Flash-photolysis of $Cl_2/CH_4/O_2$ mixtures. $P = (60-700)$ torr.	EX	298	(4.94±0.30)(9)			2
81 SAN/WAT1 $k_a + k_b$. CH_3O_2 produced by $Cl_2/CH_4/O_2$ Photolysis. UV-Absorption. Upper-limit k. $[CH_3O_2]_0 = (0.5-5.0) \times 10^{12}$ molec.cm ⁻³ . $[SO_2] = (0.76-5.66) \times 10^{16}$ molec.cm ⁻³ . $P(Total) \sim 250$ torr.	EX	298-423	≤3.01(7)			2
$CH_3O_2 + NO \rightarrow CH_3O + NO_2$ (a) $\rightarrow CH_3O_2NO$ (b) $\rightarrow HCHO + HONO$ (c)						
Methyldioxy + Nitrogen oxide (NO)						
74 SIM/HEI3 $k_a/(k_a + k_b)$.	RL	298	2.2			2/2
76 COX/DER2 k_a . Lower-limit estimate.	ES	298	≥7.23(11)			2
79 SIM/HEI k_a . Azomethane/ O_2 / SO_2 /NO photolysis. Determined relative to the reaction: $SO_2 + CH_3O_2 \rightarrow CH_3O_2SO_2$.	RN	296	1.90(12)			2 1.58
80 COX/TYN k_a . Molecular modulation-UV Absorption spectroscopy. $P = 540$ torr.	EX	298	(3.91±1.20)(12)			2
80 SAN/WAT k_a . Flash-photolysis. UV-absorption. $P = (50-700)$ torr.	EX	298	(4.28±0.84)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 PLU/RYA1 k _a . M = He. Discharge-flow. Mass-spectrometry. CH ₃ O ₂ generated by reacting Cl atom with CH ₄ in presence of O ₂ . [Cl] ₀ = (2.0-7.0) × 10 ¹¹ molec.cm ⁻³ . [O ₂] = (8.0-10.0) × 10 ¹⁵ molec.cm ⁻³ . [NO] = (0.25-3.0) × 10 ¹³ molec.cm ⁻³ . [He] = 1.9 × 10 ¹⁷ molec.cm ⁻³ .	EX	295	(5.18 ± 1.20)(12)			2
81 SIM/HEI k _a . M = CH ₄ . Flash-photolysis of Cl ₂ in presence of CH ₄ /O ₂ /NO mixtures. UV-Absorption spectroscopy. P(Total) ~ 200 torr. P(CH ₃ O ₂) ₀ = (0.7-2.0) torr. P(NO) ₀ = (11-28) mtorr. P(CH ₄) = (70-600) torr.	EX	218-365	(1.26 ± 0.60)(12)	0	-380 ± 250	2
73 SPI/VIL k _b /(k _a + k _b).	RL	298	(6.0 ± 1.0)(-1)			2/2
78 ANA/SMI2 k _a + k _b + k _c . Flash-photolysis of Azomethane/O ₂ /NO mixtures. Lower-limit k. [Azomethane] = (1.0-3.0) × 10 ¹⁷ molec.cm ⁻³ . [NO] = (0.1-1.0) × 10 ¹⁶ molec.cm ⁻³ .	ES	298	>6.02(11)			2
79 ADA/BAS1 k _a + k _b + k _c . Flash-photolysis. Kinetic spectroscopy. [Azomethane] = 5.5 × 10 ¹⁶ molec.cm ⁻³ . [O ₂] = 7.2 × 10 ¹⁶ molec.cm ⁻³ . [Ar] ~ 2.4 × 10 ¹⁸ molec.cm ⁻³ .	EX	298	(1.8 ± 0.1)(12)			2
79 PLU/RYA k _a + k _b + k _c . Flow-reactor. Mass-spectrometry. Channel (a) is predominant.	EX	295	(4.82 ± 1.20)(12)			2
81 RAV/EIS ¹⁾	EX	240-339	(3.79 ± 1.51)(12)	0	-86 ± 112	2
81 RAV/EIS ¹⁾ Nearly T-independent k (E _a ~ 0 preferred).	EX	240-339	(4.88 ± 0.96)(12)	0	0	2
¹⁾ k _a + k _b + k _c . Azomethane (or Cl ₂)/O ₂ pulsed laser-photolysis in Ar(or CH ₄) at 355 nm. Laser-induced Fluorescence. Channel (a) predominant. P(Ar) = (40-100) torr. P(CH ₄) = 50 torr. [Azomethane] = (0.5-1.6) × 10 ¹⁶ molec.cm ⁻³ . [CH ₃ O ₂] = (1.2-8.6) × 10 ¹² molec.cm ⁻³ . [O ₂] = (1.2-2.6) × 10 ¹⁷ molec.cm ⁻³ . [NO] = (0.7-4.1) × 10 ¹⁴ molec.cm ⁻³ .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{O} + \text{NO}_3^{\cdot}$ (a)						
$\rightarrow \text{HCHO} + \text{HONO}_2$ (b)						
$\rightarrow \text{CH}_3\text{OONO}_2$ (c)						
Methyldioxy + Nitrogen oxide (NO_2)						
76 COX/DER2 ($k_a + k_b + k_c$)/ k_{ref} . Approximate ratio. k_{ref} : $\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{O} + \text{NO}_2$	RL	298	$\approx 5.0(-2)$			2/2
80 ADA/BAS1 $k_a + k_b + k_c$. Azomethane Flash-photolysis. Kinetic Spectroscopy. P = (53-580) torr.	EX	298	(9.2 $\pm$ 0.4)(11)			2
73 SPI/VIL $k_c/(k_b + k_c)$.	RL	298	(7.5 $\pm$ 0.5)(-1)			2/2
80 COX/TYN ¹) P(N_2) = 540 torr.	EX	298	(9.6 $\pm$ 1.81)(11)			2
80 COX/TYN ¹) P(Ar + CH_4) = 50 torr.	EX	298	(7.23 $\pm$ 1.81)(11)			2
¹) k_c . UV-Absorption Spectroscopy.						
80 RAV/EIS ²) P(N_2) = 76 torr.	EX	298	(8.19 $\pm$ 1.39)(11)			2
80 RAV/EIS ²) P(N_2) = 722 torr.	EX	298	(2.48 $\pm$ 0.23)(12)			2
²) k_c . M = N_2 . Azomethane/ $\text{N}_2/\text{O}_2/\text{NO}_2$ photolysis. k's at other temperatures, for various N_2 pressures and concentrations of reactants also included. [Azomethane] = (0.5-2.1) molec.cm ⁻³ . [CH_3O_2] ₀ = (0.9-0.7) molec.cm ⁻³ . [NO_2] = (2.6-31.7) molec.cm ⁻³ .						
80 SAN/WAT ³) M = He.	EX	298	(5.32 $\pm$ 0.39)(11)			2
80 SAN/WAT ³) M = N_2 .	EX	298	(6.93 $\pm$ 0.60)(11)			2
80 SAN/WAT ³) M = SF_6 .	EX	298	(7.71 $\pm$ 0.96)(11)			2
³) k_c . Flash-photolysis/UV-Absorption. P = 50 torr. Other k's are given for various pressures up to to 700 torr. The k's increase with the pressure.						
$\text{CH}_3\text{O}_2 + \text{CO} \rightarrow \text{CH}_3\text{O} + \text{CO}_2$						
Methyldioxy + Carbon monoxide						
80 SAN/WAT Flash-photolysis/UV-Absorption. P = (50-700) torr. Upper-limit k.	EX	298	$\leq 4.22(6)$			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃O₂ + HCHO → CH₃OOH + CHO						
Methyldioxy + Formaldehyde						
79 SEL/WAD Di-t-butyl peroxide pyrolysis in a static system.	ES	410	≈1.2(6)			2
CH₃O₂ + CH₃O₂ → HCHO + CH₃OH + O₂ (a)						
→ CH ₃ O + CH ₃ O + O ₂ (b)						
→ CH ₃ OOCH ₃ + O ₂ (c)						
Methyldioxy						
75 ALC/MIL k _a .	ES	373	2.4(11)			2
75 PAR k _a . Unreported T assumed to be 298 K.	EX	298	1.48(11)			2
77 ALC/MIL k _a . Azomethane photolysis.	RN	373	2.4(11)			2
77 ALC/MIL k _a /k _b . Estimated ratio. Azomethane photolysis.	RL	373	(2.5±1.2)(-1)			2/2
79 SEL/WAD k _a /k _b . Di-t-butyl peroxide thermolysis. Static system. Gas-chromatography. Mass-spectrometry.	RL	410	(6.9±0.8)(-1)			2/2
80 KAN/CAL ¹⁾ k _a /k _b .	RL	298	(1.32±0.16)			2/2
80 KAN/CAL ¹⁾ k _a /k _c . Lower-limit ratio.	RL	298	≥7.0			2/2
¹⁾ Photolysis of Azomethane and Oxygen mixtures.						
75 WEA/MEA ²⁾	RL	298	5.0(-1)			2/2
75 WEA/SHO ²⁾ Azomethane photolysis. FTIR-Spectroscopy.	RL	288	5.0(1)			2/2
81 NIK/MAK ²⁾ Photooxidation of Azomethane, or Cl-atom initiated oxidation of CH ₄ in O ₂ /N ₂ . FTIR-method. P = 700 torr.	RL	297	6.0(-1)			2/2
²⁾ k _a /(k _a + k _b + k _c).						
75 ALC/MIL ³⁾	ES	373	2.3(11)			2
75 PAR ³⁾	EX	298	8.73(10)			2
77 ALC/MIL ³⁾ Azomethane photolysis.	ES	373	2.3(11)			2
77 PAR ³⁾	EX	298	(9.64±2.41)(10)			2
³⁾ k _b .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 WEA/MEA ⁴)	RL	298	4.3(-1)			2/2
75 WEA/SHO ⁴)	RL	288	4.3(-1)			2/2
Azomethane photolysis.						
81 NIK/MAK ⁴)	RL	297	3.2(-1)			2/2
Photooxidation of Azomethane, or Cl-atom, initiated oxidation of CH ₄ in O ₂ /N ₂ . FTIR-method. P = 700 torr.						
⁴) k _b /(k _a + k _b + k _c).						
75 WEA/MEA ⁵)	RL	298	7.0(-2)			2/2
75 WEA/SHO ⁵)	RL	288	7.2(-2)			2/2
Azomethane Photolysis.						
81 NIK/MAK ⁵)	RL	297	8.0(-2)			2/2
Photooxidation of Azomethane, or Cl-atom initiated oxidation of CH ₄ in O ₂ /N ₂ . FTIR-method. P = 700 torr.						
⁵) k _c /(k _a + k _b + k _c).						
75 PAR ⁶)	EX	298	(2.35±0.30)(11)			2
79 COX/TYN ⁶)	EX	298	(3.13±0.54)(11)			2
⁶) k _a + k _b .						
77 PAR	EX	298	(1.84±0.48)(11)			2
k _a + k _c .						
73 PAR/PAU ⁷)	EX	298	(1.99±0.66)(11)			2
77 HOC/GHO ⁷)	EX	295	(2.3±0.3)(11)			2
Molecular-Modulation UV-Absorption Spectrometry.						
78 ANA/SMI2 ⁷)	EX	298	(2.65±0.60)(11)			2
Azomethane/O ₂ Flash-photolysis. [Azomethane] = (1-3)×10 ¹⁷ molec.cm ⁻³ .						
79 KAN/MCQ ⁷)	ES	298	(2.4±0.1)(11)			2
Azomethane/O ₂ Flash-photolysis.						
79 SAN/SIM ⁷)	EX	298	(2.23±0.18)(11)			2
Flash-photolysis of Cl ₂ /CH ₄ /O ₂ . P = (70-600) torr.						
80 ADA/BAS2 ⁷)	EX	298	(3.5±0.3)(11)			2
Azomethane/O ₂ Flash-photolysis.						
80 SAN/WAT ⁷)	EX	298	(2.17±0.42)(11)			2
Flash-photolysis. UV-Absorption. P = (50-700) torr.						
81 SAN/WAT2 ⁷)	EX	248-417	(8.43±1.20)(10)	0	-223±41	2
CH ₃ O ₂ produced by Cl ₂ /CH ₄ /O ₂ Flash-photolysis. UV-Absorption Spectrometry. [CH ₃ O ₂] = (0.04-2.0)×10 ¹⁴ molec.cm ⁻³ . P(Total) ~ 250 torr.						
⁷) k _a + k _b + k _c .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CD}_3\text{O}_2 + \text{CD}_3\text{O}_2 \rightarrow \text{DCDO} + \text{CD}_3\text{OD} + \text{O}_2$ (a)						
$\rightarrow \text{CD}_3\text{O} + \text{CD}_3\text{O} + \text{O}_2$ (b)						
$\rightarrow \text{CD}_3\text{OOCDC}_3 + \text{O}_2$ (c)						
Methyldioxy-d ₃						
75 WEA/MEA ¹) ⁴)	RL	298	4.1(-1)			2/2
75 WEA/SHO ¹) ⁴)	RL	288	6.0(-1)			2/2
¹) $k_a/(k_a + k_b + k_c)$.						
75 WEA/MEA ²) ⁴)	RL	298	4.5(-1)			2/2
75 WEA/SHO ²) ⁴)	RL	288	2.2(-1)			2/2
²) $k_b/(k_a + k_b + k_c)$.						
75 WEA/MEA ³) ⁴)	RL	298	1.4(-1)			2/2
75 WEA/SHO ³) ⁴)	RL	288	1.8(-1)			2/2
³) $k_c/(k_a + k_b + k_c)$.						
⁴) Azomethane-d ₆ Photolysis.						
$\text{CH}_3\text{O}_2 + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{O} + \triangle\text{O}$						
Methyldioxy + Ethene						
80 SEL/WAD	EX	410	(1.2±0.7)(3)			2
Di-t-Butyl peroxide oxidation.						
Static system.						
Gas-chromatography.						
Mass-spectrometry.						
81 NIK/MOS	EX	593	(4.6±0.9)(7)			2
CH_3O_2 generated by Thermolysis of Di-t-butyl						
peroxide [P(Total) = (50-400) torr.], or of						
Azomethane [P(Total) = (50-60) torr.],						
in presence of O_2 and $\text{CH}_2=\text{CH}_2$.						
Gas-chromatography.						
$\text{CH}_3\text{O}_2 + \text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow \text{CH}_3\text{O} + \text{CH}_3 + \text{CO}_2 + \text{O}_2$						
Methyldioxy + Ethyldioxy, 1-oxo-						
80 ADD/BURR	DE	302	1.81(12)			2 2.0
Cl_2 modulated photolysis, in presence						
of CH_3CHO and O_2 .						
Computer simulation data-fit.						
$\text{CH}_3\text{O}_2 + \text{CH}_3\text{N}=\text{NCH}_3 \rightarrow \text{products (overall)}$						
Methyldioxy + Diazene, dimethyl- (Azomethane)						
79 KAN/MCQ	EX	298	(8.0±3.0)(7)			2
Azomethane/ O_2 Flash-photolysis.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{O}_2 + (\text{CH}_3)_2\text{CHO}_2 \rightarrow \text{CH}_3\text{OH} + (\text{CH}_3)_2\text{CO} + \text{O}_2$ Methyldioxy + Ethyldioxy, 1-methyl- 77 ALC/MIL Azomethane photolysis. Same data given in 75 ALC/MIL.	ES	373	6.2(11)			2	
$\text{CH}_3\text{O}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow \text{CH}_3\text{O} + \text{CH}_3\text{C}(\text{CH}_3)_2\text{O}$ Methyldioxy + 1-Propene, 2-methyl- 80 SEL/WAD Di-t-Butyl peroxide oxidation. Static system. Gas-chromatography. Mass-spectrometry.	EX	410	(9.8±1.6)(3)			2	
$\text{CH}_3\text{O}_2 + (\text{CH}_3)_3\text{CO}_2 \rightarrow \text{CH}_3\text{O} + (\text{CH}_3)_3\text{CO} + \text{O}_2$ (a) $\rightarrow \text{HCHO} + (\text{CH}_3)_3\text{COH} + \text{O}_2$ (b) Methyldioxy + Ethyldioxy, 1,1-dimethyl- 75 FAR $k_a = k_b$. Unreported T assumed to be 298 K. 81 KIR/FAR ¹⁾ 81 KIR/FAR ¹⁾ ¹⁾ k_a/k_b . Azo-t-butane/ O_2 photolysis. Gas-chromatography. Approximate rate ratios.	EX	298	(3.01±1.51)(10)			2	
$\text{CH}_3\text{O}_2 + \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{O} + \text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{O}$ Methyldioxy + 1-Butene, 2-methyl- 80 OSB/WAD Di-t-Butyl peroxide oxidation. Static system. Gas-chromatography. Mass-spectrometry.	EX	373-403	3.98(11)	0	6351±650	2	5.25
$\text{CH}_3\text{O}_2 + (\text{CH}_3)_2\text{C}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{O} + \text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{O}$ Methyldioxy + 2-Butene, 2-methyl- 80 OSB/WAD Di-t-Butyl peroxide oxidation. Static system. Gas-chromatography. Mass-spectrometry.	EX	373-403	1.44(11)	0	5100±433	2	3.09

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k(k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
$\text{CH}_3\text{O}_2 + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{O} + \text{H}_3\text{C}-\text{C}(\text{O})-\text{CH}_3$						
Methyldioxy + 2-Butene, 2,3-dimethyl-						
80 OSB/WAD	EX	373-403	1.38(11)	0	4378±337	2 2.09
Di-t-Butyl peroxide oxidation. Static system.						
Gas-chromatography. Mass-spectrometry.						
$\text{CH}_3\text{O}_2 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{OOH} + (\text{CH}_3)_2\text{CHC}(\text{CH}_3)_2$						
Methyldioxy + Butane, 2,3-dimethyl-						
75 ALC/MIL	ES	373	1.6(5)			2
77 ALC/MIL	ES	373	1.6(5)			2
Azomethane photolysis.						
$\text{CH}_3\text{O}_2 + (\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2 \rightarrow \text{HCHO} + (\text{CH}_3)_2\text{CHC}(\text{OH})(\text{CH}_3)_2 + \text{O}_2$						
Methyldioxy + Propyldioxy, 1,1,3-trimethyl-						
77 ALC/MIL	ES	373	2.4(11)			2
Azomethane photolysis.						
$\text{HOCH}_2\text{O} + \text{O}_2 \rightarrow \text{HCOOH} + \text{HO}_2$						
Methoxy, hydroxy- + Oxygen molecule						
82 VEY/RAY	DE	298	(2.11±0.96)(10)			2
HCHO/O ₂ /NO Flash-photolysis.						
Computer simulation data-fit.						
[HCHO] ₀ = (2-30) torr.						
[O ₂] ₀ = (2.5-45) torr.						
[NO] ₀ = (15-200) torr.						
$\text{HOCH}_2\text{O} + \text{NO} \rightarrow \text{HOCH}_2\text{ONO} \quad (\text{a})$ $\rightarrow \text{HNO} + \text{HCOOH} \quad (\text{b})$						
Methoxy, hydroxy- + Nitrogen oxide (NO)						
82 VEY/RAY	DE	298	(2.41±1.14)(13)			2
k _a + k _b . HCHO/O ₂ /NO flash-photolysis.						
Computer simulation data-fit.						
[O ₂] ₀ = (2.5-45) torr.						
[HCHO] ₀ = (2-30) torr.						
[NO] ₀ = (15-200) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
HOCH₂O₂ → HO₂ + HCHO							
Methyldioxy, hydroxy-							
79 SU/CAL3 Cl ₂ /HCHO/synthetic air photolysis. FTIR-Spectroscopy. P(Total) ~ 700 torr.	ES	298	1.5				1
82 VEY/RAY HCHO/O ₂ /NO flash-photolysis. Data-fit. [O ₂] ₀ = (2.5-45) torr. [NO] ₀ = (15-200) torr. [HCHO] ₀ = (2-30) torr.	ES	298	3.0(1)				1
HOCH₂O₂ + NO → HOCH₂O + NO₂							
Methyldioxy, hydroxy- + Nitrogen oxide (NO)							
82 VEY/RAY HCHO/O ₂ /NO flash-photolysis. Data-fit. [O ₂] ₀ = (2.5-445) torr. [NO] ₀ = (15-200) torr. [HCHO] ₀ = (2-30) torr.	ES	298	3.37(12)				2
HOCH₂O₂ + HOCH₂O₂ → HOCH₂O + HOCH₂O + O₂							
Methyldioxy, hydroxy-							
79 SU/CAL3 Cl ₂ /HCHO/synthetic air photolysis. FTIR-Spectroscopy. P(Total) ~ 700 torr.	ES	298	7.23(10)				2
CH₃OH (+ M) → CH₃ + OH (+ M)							
Methanol							
75 BOW2 M = Ar. Reflected shock waves. Best data-fit. [Ar] = (5.7-17.0) × 10 ¹⁸ molec.cm ⁻³ . [CH ₃ OH] = 1.3 × 10 ¹⁷ molec.cm ⁻³ . [O ₂] = 2.5 × 10 ¹⁷ molec.cm ⁻³ .	ES	1545-2180	4.0(15)	0	34200		2
81 TSU/KAT ¹) Total conc. = 6.0 × 10 ¹⁸ molec.cm ⁻³ .	EX	1500-1900	6.0(12)	0	37288		1
81 TSU/KAT ¹) Total conc. = 3.0 × 10 ¹⁹ molec.cm ⁻³ .	EX	1500-1900	3.5(13)	0	37769		1
81 TSU/KAT ¹) Total conc. = 6.0 × 10 ¹⁹ molec.cm ⁻³ .	EX	1500-1900	8.7(13)	0	38251		1
81 TSU/KAT ¹) Limiting high-pressure k. Tentative.	EX	1500-1900	2.0(18)	0	47510		1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 TSU/KAT ¹⁾ Limiting low-pressure k. Tentative. ¹⁾ M = Ar. CH ₃ /O ₂ Thermal oxidation behind reflected shock-waves. UV-absorption. IR-emission. Same data given in 81 TSU/HAS.	EX	1500-1900	9.0(18)	0	40536	2
82 SPI/WAG ²⁾ Limiting high-pressure k.	EX	1600-2100	9.4(15)	0	45227	1
82 SPI/WAG ²⁾ Limiting low-pressure k. ²⁾ Methanol Thermolysis behind reflected shock-waves. Total conc. = (0.1-3.8)x10 ¹⁹ molec.cm ⁻³ . [CH ₃ OH] ₀ = (0.1-3.0)x10 ¹⁶ molec.cm ⁻³ .	EX	1600-2100	2.0(17)	0	34441	2
CS ₂ (+ M) → CS + S (+ M)						
Carbon disulfide						
74 TRA ¹⁾ Shock-tube. Unspecified high-T range.	EX	¹⁾	6.76(14)	0	35984±705	2
80 SAI/TOR M = Ar. Thermolysis behind reflected shock-waves. [CS ₂] = (0.9-2.4)x10 ¹⁶ molec.cm ⁻³ . Total Conc. = (2.0-4.8)x10 ¹⁶ molec.cm ⁻³ .	EX	2000-2900	2.51(14)	0	37393±3271	2 3.16
COS (+ M) → products						
Carbon oxide sulfide						
74 TRA ¹⁾ Shock-tube. Unspecified high-T range.	EX	¹⁾	8.32(14)	0	31706±654	2
CH ₃ S + CH ₃ S → HCBS + CH ₃ SH (a) → CH ₃ SSCH ₃ [†] (b)						
Methylthio						
73 TYC/KNI ¹⁾ k _a /k _b .	RL	298	4.0(-2)			2/2
73 TYC/KNI ¹⁾ k _a .	RN	298	9.8(11)			2
73 TYC/KNI ¹⁾ k _b .	RN	298	2.4(13)			2
¹⁾ Hg-photosensitized CH ₃ SH decomposition.						
CH ₃ S + #172 → CH ₃ S ₂ + CH ₂ =CH ₂						
Methyl, mercapto- + Thiirane (Ethylene episulfide)						
72 JAK/AHM	ES	304-478	~3.16(11)	0	~4429	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CN (+ M) → C + N (+ M)							
Cyanogen							
76 SLA M = Ar.	EX	4400-1300	(1.2±0.4)(14)	0	70961±5536	2	
CN(v=n) + O₂ → NCO + O							
Cyanogen + Oxygen molecule							
72 BUL/COO1 ¹⁾ v = 0.	EX	303	(6.77±0.15)(12)			2	
72 BUL/COO1 ¹⁾ v = 0.	EX	375	(6.34±0.22)(12)			2	
72 BUL/COO1 ¹⁾ v = 1.	EX	303	(7.6±0.2)(12)			2	
72 BUL/COO1 ¹⁾ v = 2.	EX	303	(9.26±0.22)(12)			2	
72 BUL/COO1 ¹⁾ v = 3.	EX	303	(9.83±0.31)(12)			2	
72 BUL/COO1 ¹⁾ v = 4.	EX	303	(1.17±0.35)(13)			2	
72 BUL/COO1 ¹⁾ v = 4.	EX	375	(1.11±0.06)(13)			2	
¹⁾ Possible small negative E _a .							
72 SCH/WOL2 k decreasing to 1.8x10 ¹² cm ³ mol ⁻¹ s ⁻¹ between v=0 and v=6. Unreported T assumed 298 K.	EX	298	4.7(12)			2	
73 SCH/SCH1 k(v=7) = 1.58x10 ¹² cm ³ mol ⁻¹ s ⁻¹ . k decreases monotonically from v=0 to v=7.	EX	298	6.31(12)			2	
74 SCH/SCH v = 0.	EX	299-388	3.16(13)	0	503	2	
75 ALB/HOY v = 0.	EX	718-1111	(3.2±1.0)(13)	0	505±168	2	
CN + H₂ → HCN + H							
Cyanogen + Hydrogen molecule							
74 SCH/SCH	EX	298-388	6.31(13)	0	2667	2	
75 ALB/HOY	EX	718-1111	(6.0±2.0)(13)	0	2670±301	2	
77 SCH/WAG	EX	259-396	(6.0±2.0)(13)	0	2670±301	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CN(v=n) + NO(v'=0) → N ₂ + CO (a)						
→ CN(v=n-1) + NO(v'=1) (b)						
CN(v=n) + NO (+ M) → NOCN (+ M) (c)						
Cyanogen + Nitrogen oxide (NO)						
75 MUL/PHI	ES	1500	7.3(12)			2
k _a . n = 0.						
78 LAM/DUG ¹)	EX	300	(7.23±3.61)(10)			2
k _a . n = 0.						
78 LAM/DUG ¹)	EX	300	(1.57±0.30)(11)			2
k _a + k _b .						
n = 1.						
78 LAM/DUG ¹)	EX	300	(2.79±0.51)(17)			3
k _c . n = 0.						
78 LAM/DUG ¹)	EX	300	(1.09±0.40)(17)			3
k _c . n = 1.						
¹) M = Ar.						
Flash-photolysis.						
Laser-induced fluorescence.						
CN + CO ₂ → CNO + CO						
Cyanogen + Carbon dioxide						
75 HAY/IVE	EX	1830-2400	(3.7±0.4)(12)	0	0	2
CN(v=n) + CH ₄ → HCN + CH ₃						
Cyanogen + Methane						
71 BUL/COO ¹)	EX	300	(4.46±0.1)(13)			2
n = 0.						
CN Absorption band: 0,0.						
71 BUL/COO ¹)	EX	300	(5.0±0.2)(11)			2
n = 0.						
CN Absorption band: 4,4.						
¹) Radiolysis of C ₂ N ₂ + Ar.						
72 BUL/COO2	EX	300-377	1.29(13)	0	1006±96	2
n = 0.						
74 SCH/SCH	EX	298-388	3.16(13)	0	1459	2
n = 0.						
77 SCH/WAG	EX	259-396	(6.0±3.0)(12)	0	866±301	2
n = 0.						
77 SCH/WAG	EX	298	7.0(11)			2
n = 1.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CN + CD₄ → DCN + CD₃						
Cyanogen + Methane-d ₄						
72 BUL/COO2 CN(0,0) band.	EX	300	(2.4±0.4)(11)			2
72 BUL/COO2 CN(4,4) band.	EX	300	(3.5±0.2)(11)			2
CN + COS → SCN + CO						
Cyanogen + Carbon oxide sulfide						
79 ADD/LEI Time-resolved spectrophotometry. Lower-limit k.	EX	295	≥1.81(13)			2
CN(v=n) + CH≡CH → products						
Cyanogen + Ethyne						
77 SCH/WAG v = 0.	EX	259-396	(3.0±1.0)(13)	0	0	2
77 SCH/WAG v = 1. Lower-limit k.	EX	298	≥1.5(14)			2
CN + CH₂=CH₂ → CH₂CH₂CN (a) → any other products (b)						
Cyanogen + Ethene						
71 BUL/COO ¹ CN Absorption band: 0,0.	EX	300	(1.16±0.15)(14)			2
71 BUL/COO ¹ CN Absorption band: 4,4.	EX	300	(1.35±0.20)(14)			2
¹) k _a . Radiolysis of C ₂ N ₂ + Ar.						
77 SCH/WAG ² v = 0.	EX	259-396	(3.0±0.5)(13)	0	0	2
77 SCH/WAG ² v=1.	EX	298	6.5(13)			2
²) k _{overall} .						
CN + CH₃CH₃ → HCN + CH₃CH₂						
Cyanogen + Ethane						
71 BUL/COO CN Absorption bands: 0,0 and 4,4. Radiolysis of C ₂ N ₂ + Ar.	EX	300	(1.45±0.10)(13)			2
72 BUL/COO2	EX	300-415	2.40(13)	0	192	2
72 BUL/COO2 B = 0 assumed.	EX	300-415	1.48(13)	0	0	2
74 SCH/SCH	EX	298	7.94(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CN + NCCN → [C₃N₃]						
Cyanogen + Ethanedinitrile						
72 BUL/COO1	EX	300-377	5.62(11)	0	1576	2
CN + CH₃CH=CH₂ → products						
Cyanogen + 1-Propene						
71 BUL/COO	EX	300	(1.6±0.2)(14)			2
CN Absorption band: 0,0. C ₂ N ₂ /Ar Radiolysis.						
CN + CH₃CH₂CH₃ → HCN + CH₃CH₂CH₂ (a) → HCN + (CH₃)₂CH (b)						
Cyanogen + Propane						
72 BUL/COO2	EX	300	(3.2±0.5)(13)			2
k _a + k _b .						
CN + CH₂=CHCH=CH₂ → products						
Cyanogen + 1,3-Butadiene						
71 BUL/COO	EX	300	(2.6±0.3)(14)			2
CN Absorption band: 0,0. C ₂ N ₂ /Ar Radiolysis.						
NCO + O₂ → NO + CO₂						
Cyanato + Oxygen molecule						
74 SCH/SCH	EX	298	7.94(11)			2
HCN (+ M) → H + CN (+ M)						
Hydrocyanic acid						
76 ROT/JUS	EX	2200-2700	5.72(16)	0	58940	2
M = Ar. Thermolysis behind shock-waves.						
80 ROT	EX	2200-2700	5.72(16)	0	59060	2
M = Ar. HCN Thermolysis behind shock-waves.						
Resonance-absorption.						
Same data given in 79 ROT/JUS1.						
82 SZE/HAN	EX	3570-5036	4.07(17)	0	44740±1060	2 1.29
M = Ar. HCN Thermolysis behind incident shock-waves in Ar. P = (128-218) torr.						
CH₃NH₂ (+ M) → CH₃ + NH₂ (+ M)						
Methanamine						
79 DOR/PCH ¹⁾	EX	1275-2400	6.92(10)	0	24233	1
Limiting high-pressure k.						
79 DOR/PCH ¹⁾	EX	1275-2400	3.16(13)	0	17685	2
Limiting low-pressure k.						
¹⁾ Reflected shock-waves. IR-emission techniques.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{N}=\text{N} \rightarrow \text{CH}_3 + \text{N}_2$ Diazenyl, methyl- 76 VID/WIL	EX	295	$\geq 3.0(6)$			1	
$\text{CH}_3\text{NHNH}_2 \rightarrow \text{CH}_2=\text{NH} + \text{NH}_3$ (a) $\rightarrow \text{CH}_3\text{N}=\text{NH} + \text{H}_2$ (b) Hydrazine, methyl- 72 GOL/SOL k_a . RRKM fit of experimental data.	EX	943-1263	1.58(13)	0	27177	1	
72 GOL/SOL k_b . RRKM fit of experimental data.	EX	943-1263	3.16(13)	0	28686	1	
$\text{NH}_2\text{CO} (+\text{M}) \rightarrow \text{NH}_2 + \text{CO} (+\text{M})$ Amidogen, formyl- 73 YOK/BAC M = HCONH_2 . Limiting high-pressure k.	RN	578	$(5.9 \pm 2.0)(12)$			1	
73 YOK/BAC k_o . M = HCONH_2 . Low-pressure.	RN	578	$(1.04 \pm 0.35)(17)$			2	
$\text{NH}_2\text{CO} + \text{NH}_2\text{CO} \rightarrow \text{NH}_2\text{COCOCONH}_2$ (a) $\rightarrow \text{HNCO} + \text{HCONH}_2$ (b) Amidogen, formyl- 73 YOK/BAC $k_a + k_b$.	EX	578	$(3.1 \pm 1.0)(13)$			2	
$\text{CH}_3\text{NO}^\dagger \rightarrow \text{CH}_3 + \text{NO}$ Methane, nitroso- 74 TIT/BAL $\text{CH}_3\text{NO}^\dagger$ generated by reacting CH_3 with NO.	ES	443	2.0(7)			1	
$\text{CH}_3\text{ONO} (+\text{M}) \rightarrow \text{HCHO} + \text{HNO} (+\text{M})$ (a) $\rightarrow \text{CH}_3\text{O} + \text{NO} (+\text{M})$ (b) Nitrous acid methyl ester 75 BAT/MCC k_a .	ES	393-473	1.0(10)	0	16004	1	
77 BAT/MIL3 k_a .	ES	440-473	3.98(13)	0	19376 $\pm$ 503	1	3.98

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
74 BAT/MIL k_b .	ES	393-473	6.31(15)	0	20735±503	1	2.51
75 BAT/MCC k_b .	ES	393-473	6.31(15)	0	20735±503	1	2.51
77 BAT/MIL3 k_b .	ES	440-473	6.31(15)	0	20745±503	1	3.98
75 MAL/GAN M = Ar. Incident and reflected shockwaves. P = (0.8-5) atm.	EX	715-1118	2.29(16)	0	15299±428	2	1.66
 $\text{CH}_3\text{NO}_2 (+\text{M}) \rightarrow \text{CH}_3 + \text{NO}_2 (+\text{M})$ Methane, nitro-							
72 GLA/TRO M = Ar. Limiting high-pressure k.	EX	900-1400	1.78(16)	0	29441±252	1	
72 GLA/TRO M = Ar. Low-pressure k.	EX	900-1370	1.26(17)	0	21137	2	
 $\text{CH}_3\text{ONO}_2 \rightarrow \text{CH}_3\text{O} + \text{NO}_2$ Nitric acid methyl ester							
77 BAT/MIL3	ES	440-473	5.01(15)	0	20382±503	1	3.98
 $\text{CH}_3\text{O}_2\text{NO}_2 (+\text{M}) \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2 (+\text{M})$ Peroxynitric acid methyl ester							
82 BAH/SIM ¹⁾ Experimental k. P ~ 350 torr.	EX	256-268	6.0(15)	0	10619±755	1	
82 BAH/SIM ¹⁾ Optimization based on combination of the above experimental data with k_{-1} and thermodynamic data.	DE	256-268	(6.0±3.0)(15)	0	10720±151	1	
82 BAH/SIM ¹⁾ Limiting high-pressure k.	CO	256-268	2.1(16)	0	10921±151	1	
82 BAH/SIM ¹⁾ Limiting low-pressure k. Both limiting k values are evaluations based on the P-dependence of k_{-1} .	DE	256-268	2.0(20)	0	10141±151	2	
 ¹⁾ $\text{CH}_3\text{O}_2\text{NO}_2$ decomposition in a Pyrex reaction cell with vacuum system. UV-spectrometry. $\text{CH}_3\text{O}_2\text{NO}_2$ generated by $\text{Cl}_2/\text{O}_2/\text{CH}_4/\text{NO}_2$ photolysis.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$C_2(X^1\Sigma_g^+ = A^3\Pi_g) (+M) \rightarrow C + C (+M)$							
Carbon dimer							
75 BEC/MAC M = Ar. Shock-wave pyrolysis of CH $\equiv$ CH in Ar.	EX	4860-6920	3.71(14)	0	69885 $\pm$ 7097	2	1.86
$C_2(X^1\Sigma_g^+) + O_2 \rightarrow CO^* + CO$ (a) $\rightarrow$ any other products (b)							
Carbon dimer + Oxygen molecule							
80 REI/MAN1 k_a . CH $_2$ =CHCN/O $_2$ Multiphoton dissociation. CO* is in an electronically excited triplet state.	EX	300	(1.81 $\pm$ 0.12)(12)			2	
79 PAS/MCD $k_{overall}$. CF $_3$ C $\equiv$ CF $_3$ Multiphoton laser photodissociation. Laser-induced fluorescence.	EX	298	(1.70 $\pm$ 0.05)(12)			2	
80 MAN/REI $k_{overall}$. CH $_2$ =CN or CHCl=CCl $_2$ Multiphoton laser dissociation in a fluorescence chamber.	CO	298	1.63(12)			2	
82 PIT/PAS ¹⁾ C $_2$ (X $^1\Sigma_g^+$) reacts as fast as C $_2$ (a $^3\Pi_u$).	EX	300-600	(6.44 $\pm$ 1.51)(12)	0	337 $\pm$ 81	2	
82 PIT/PAS ¹⁾ C $_2$ (X $^1\Sigma_g^+$) reacts much faster than C $_2$ (a $^3\Pi_u$). ¹⁾ $k_{overall}$. Dye-laser induced fluorescence. C $_2$ produced by multiphoton UV-photolysis of CF $_3$ C $\equiv$ CF $_3$.	EX	300-600	(2.00 $\pm$ 0.60)(13)	0	604 $\pm$ 101	2	
$C_2(a^3\Pi_u) + O_2 \rightarrow CO(A^1\Pi) + CO$ (a) $\rightarrow CO^* + CO$ (b)							
Carbon dimer + Oxygen molecule							
79 FIL/HAN k_a . Laser-induced fluorescence.	EX	298	2.05(12)			2	
80 REI/MAN1 k_b . CH $_2$ =CHCN/O $_2$ Multiphoton dissociation. CO* is an electronically excited triplet.	EX	300	(1.81 $\pm$ 0.12)(12)			2	
79 DON/PAS $k_{overall}$. CH $\equiv$ CH Multiphoton photolysis. Dye-laser induced fluorescence. P(N $_2$) = (10-45) torr.	EX	298	(1.78 $\pm$ 0.04)(12)			2	
80 MAN/REI $k_{overall}$. CH $_2$ =CHCN or CHCl=CCl $_2$ Multiphoton dissociation in a fluorescence chamber.	CO	298	1.63(12)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 PIT/PAS k_{overall} $C_2(a^3\Pi_u)$ is assumed to react as fast as $C_2(X^1\Sigma_g^+)$. Dye-laser induced fluorescence. C_2 produced by Multiphoton Photolysis of $CF_3\equiv CCF_3$.	EX	300-600	(6.44±1.51)(12)	0	337±81	2
$C_2(X^1\Sigma_g^+) + H_2O \rightarrow \text{products}$ Carbon dimer + Water						
80 REI/MAN2 $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation. Laser-induced fluorescence. Upper-limit k.	EX	300	<1.81(10)			2
$C_2(a^3\Pi_u) + H_2O \rightarrow \text{products}$ Carbon dimer + Water						
80 REI/MAN2 $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation. Laser-induced fluorescence. Upper-limit k.	EX	300	<1.81(10)			2
$C_2(X^1\Sigma_g^+) + N_2 \rightarrow \text{products}$ Carbon dimer + Nitrogen molecule						
80 REI/MAN2 $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation. Laser-induced fluorescence. Upper-limit k.	EX	300	<1.81(10)			2
$C_2(a^3\Pi_u) + N_2 \rightarrow \text{products}$ Carbon dimer + Nitrogen molecule						
80 REI/MAN2 $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation. Laser-induced fluorescence. Upper-limit k.	EX	300	<1.81(10)			2
$C_2(X^1\Sigma_g^+) + NO \rightarrow CN(X^2\Sigma^+) + CO$ (a) $\rightarrow CN(A^2\Pi) + CO$ (b) Carbon dimer + Nitrogen oxide (NO)						
82 LE k_a . Premixed fuel-rich $CH=CH/NO$ flames, at 250-600 nm. P = 80 torr.	ES	2700	3.6(14)			2
80 REI/MAN2 $k_a + k_b$. $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation. Laser-induced fluorescence.	EX	300	1.26(14)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$C_2(a^3\Pi_u) + NO \rightarrow CN(X^2\Sigma^+) + CO$ (a)						
$\rightarrow CN(B^2\Sigma^+) + CO$ (b)						
$\rightarrow CN(A^2\Pi) + CO$ (c)						
$\rightarrow CN(X^2\Sigma^+) + CO(a^3\Pi)$ (d)						
Carbon dimer + Nitrogen oxide (NO)						
79 REI/MAN ¹⁾ k determined by using LIF to monitor $C_2(a^3\Pi_u)$.	EX	298	(4.40±0.54)(13)			2
79 REI/MAN ¹⁾ k determined from $CN(B^2\Sigma^+ \rightarrow X^2\Sigma^+)$ chemiluminescence.	EX	298	(4.52±0.18)(13)			2
79 REI/MAN ¹⁾ k determined from $CN(A^2\Pi \rightarrow X^2\Sigma^+)$ chemiluminescence.	EX	298	(4.40±0.18)(13)			2
¹⁾ $k_a + k_b + k_c + k_d$. Ethylene, or Vinyl cyanide Multiple-photon dissociation. Time-resolved Chemiluminescence. Laser-induced Fluorescence. $P(CH_2=CHCN) = (1-10)$ mtorr. $P(CH_2=CH_2) = (1-10)$ mtorr. $P(Ar) = (50-500)$ mtorr.						
$C_2(X^1\Sigma_g^+) + CO_2 \rightarrow$ products						
Carbon dimer + Carbon dioxide						
80 REI/MAN2 $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation. Laser-induced fluorescence. Upper-limit k.	EX	300	<1.81(10)			2
$C_2(a^3\Pi_u) + CO_2 \rightarrow$ products						
Carbon dimer + Carbon dioxide						
80 REI/MAN2 $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation. Laser-induced fluorescence. Upper-limit k.	EX	300	<1.81(10)			2
$C_2(X^1\Sigma_g^+) + CH_4 \rightarrow CH=C + CH_3$ (a)						
$\rightarrow CH_3C\equiv CH$ (b)						
Carbon dimer + Methane						
79 PAS/MCD k_a . $CF_3C\equiv CCF_3$ Multiphoton laser photodissociation. Laser-induced fluorescence.	EX	298	(1.13±0.03)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, σ B-B(ref)	k, A k err. units factor
82 PIT/PAS k_b . Dye-laser induced fluorescence. C_2 produced by multiphoton UV-Photolysis of $CF_3C\equiv CCF_3$.	EX	300-600	(3.04 $\pm$ 0.09)(13)	0	297 $\pm$ 10	2
80 REI/MAN2 $k_{overall}$. $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation. Laser-induced fluorescence.	EX	300	(1.02 $\pm$ 0.12)(13)			2
$C_2(a^3\Pi_u) + CH_4 \rightarrow$ products						
Carbon dimer + Methane						
79 DON/PAS $CH\equiv CH$ Multiphoton photolysis. Dye-laser induced fluorescence. Upper-limit k. $P(CH_4) = (0-250)$ torr. $P(N_2) = (0-10)$ torr.	EX	298	<6.02(7)			2
80 PAS/BAR $CF_3C\equiv CCF_3$ Multiphoton UV-photolysis. Dye-laser induced fluorescence. $P(CF_3C\equiv CCF_3) = (1.5-4.0)$ mtorr. $P(CH_4) \sim (10-170)$ torr.	EX	337-605	(9.94 $\pm$ 1.20)(12)	0	2805 $\pm$ 55	2
80 REI/MAN2 $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation. Laser-induced fluorescence. Upper-limit k.	EX	300	<1.81(10)			2
$C_2(X^1\Sigma_g^+) + CH\equiv CH \rightarrow$ products						
Carbon dimer + Ethyne						
80 REI/MAN2 $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation. Laser-induced fluorescence.	EX	300	(2.59 $\pm$ 0.24)(14)			2
$C_2(a^3\Pi_u) + CH\equiv CH \rightarrow$ products						
Carbon dimer + Ethyne						
79 DON/PAS $CH\equiv CH$ Multiphoton photolysis Dye-laser induced fluorescence. P-independent.	EX	298	(5.78 $\pm$ 0.18)(13)			2
$C_2(X^1\Sigma_g^+) + CH_2=CH_2 \rightarrow$ products						
Carbon dimer + Ethene						
79 PAS/MCD $CF_3C\equiv CCF_3$ Multiphoton laser photodissociation. Laser-induced fluorescence.	EX	298	(1.96 $\pm$ 0.03)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
$C_2(a^3\Pi_u) + CH_2=CH_2 \rightarrow$ products						
Carbon dimer + Ethene						
79 DON/PAS CH=CH Multiphoton photolysis. Dye-laser induced fluorescence. P(N ₂) = (10-60) torr.	EX	298	(8.67±0.36)(13)			2
81 PAS/PIT CF ₃ C≡CCF ₃ or C ₆ H ₆ Multiphoton laser dissociation. Laser-induced fluorescence.	EX	300-600	(7.23±0.96)(13)	0	-5±46	2
$C_2(X^1\Sigma_g^+) + CH_3CH_3 \rightarrow CH\equiv C + CH_3CH_2$						
Carbon dimer + Ethane						
79 PAS/MCD CF ₃ C≡CCF ₃ Multiphoton laser photodissociation. Laser-induced fluorescence.	EX	298	(9.58±0.30)(13)			2
$C_2(a^3\Pi_u) + CH_3CH_3 \rightarrow CH\equiv C + CH_3CH_2$						
Carbon dimer + Ethane						
79 DON/PAS CH=CH Multiphoton photolysis. Dye-laser induced fluorescence. P(N ₂) = (10-60) torr.	EX	298	(7.83±0.36)(11)			2
81 PAS/PIT CF ₃ C≡CCF ₃ or C ₆ H ₆ Multiphoton laser dissociation. Laser-induced fluorescence.	EX	300-600	(1.46±0.06)(13)	0	919±15	2
$C_2(X^1\Sigma_g^+) + CH_2=CHCN \rightarrow$ products						
Carbon dimer + 2-Propenenitrile (Acrylonitrile)						
80 REI/MAN2 CH ₂ =CHCN or CHCl=CCl ₂ Multiphoton dissociation. Laser-induced fluorescence.	EX	300	(2.65±0.18)(14)			2
$C_2(a^3\Pi_u) + CH_2=CHCN \rightarrow$ products						
Carbon dimer + 2-Propenenitrile (Acrylonitrile)						
80 REI/MAN2 CH ₂ =CHCN or CHCl=CCl ₂ Multiphoton dissociation. Laser-induced fluorescence.	EX	300	(3.43±0.24)(13)			2
$C_2(X^1\Sigma_g^+) + CH_2=C=CH_2 \rightarrow$ products						
Carbon dimer + 1,2-Propadiene						
80 REI/MAN2 CH ₂ =CHCN or CHCl=CCl ₂ Multiphoton dissociation. Laser-induced fluorescence.	EX	300	(2.83±0.24)(14)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$C_2(a^3\Pi_u) + CH_2=C=CH_2 \rightarrow$ products						
Carbon dimer + 1,2-Propadiene						
80 REI/MAN2	EX	300	(1.57±0.12)(14)			2
$CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation.						
Laser-induced fluorescence. Upper-limit k.						
$C_2(X^1\Sigma_g^+) + CH_3CH_2CH_3 \rightarrow$ products						
Carbon dimer + Propane						
80 REI/MAN2	EX	300	(1.99±0.12)(14)			2
$CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation.						
Laser-induced fluorescence. Upper-limit k.						
$C_2(a^3\Pi_u) + CH_3CH_2CH_3 \rightarrow CH\equiv C + CH_3CH_2CH_2$ (a)						
$\rightarrow CH\equiv C + (CH_3)_2CH$ (b)						
Carbon dimer + Propane						
81 PAS/PIT	EX	300-600	(1.11±0.10)(13)	0	97±36	2
$k_a + k_b$.						
$CF_3C\equiv CCF_3$ Multiphoton laser dissociation.						
Laser-induced fluorescence.						
80 REI/MAN2	EX	300	(1.00±0.06)(14)			2
$k_{overall}$.						
$CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation.						
Laser-induced fluorescence.						
$C_2(a^3\Pi_u) + CH_3CH_2CH_2CH_3 \rightarrow CH\equiv C + CH_3CH_2CH_2CH_2$ (a)						
$\rightarrow CH\equiv C + CH_3CH_2CHCH_3$ (b)						
Carbon dimer + Butane						
81 PAS/PIT	EX	300-600	(2.95±0.30)(13)	0	71±41	2
$CF_3C\equiv CCF_3$ or C_6H_6 Multiphoton laser dissociation.						
Laser-induced fluorescence.						
$C_2O + CH\equiv CH \rightarrow$ products						
Carbon oxide (C_2O) + Ethyne						
80 DON/PIT	EX	298	<6.02(9)			2
C_3O_2 photodissociation at 266 nm. Dye-laser induced fluorescence. Upper-limit k.						
$C_2O + CH_2=CH_2 \rightarrow$ products						
Carbon oxide (C_2O) + Ethene						
80 DON/PIT	EX	298	<6.02(9)			2
C_3O_2 photodissociation at 266 nm. Dye-laser induced fluorescence. Upper-limit k.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	E, B-B(ref)	k, A k err. units factor
C₂O + (CH₃)₂C=CH₂ → products						
Carbon oxide (C ₂ O) + 1-Propene, 2-methyl-						
80 DON/PIT	EX	298	(6.75±0.30)(10)			2
C ₃ O ₂ Laser photodissociation at 266 nm. Dye-laser induced fluorescence.						
CH≡C (+ M) → C₂ + H (+ M)						
Ethyne						
75 BEC/MAC ¹⁾	DE	4860-6920	3.61(15)	0	71930	2
M = Ar.						
75 BEC/MAC ¹⁾	DE	4860-6920	6.02(13)	0	14554	2
M = H.						
¹⁾ Shock-wave pyrolysis. CH≡CH in Ar. Best-fit.						
CH≡C + O₂ → products						
Ethyne + Oxygen molecule						
75 LAN/WAG	EX	320	≈3.3(12)			2
Discharge-flow. Mass-spectrometry. P = 4.1 torr.						
82 REN/SRO	EX	300	(1.26±0.18)(13)			2
M = He or Ar. Vacuum chamber. CH≡C produced by Laser-Photolysis of CH≡CH, CH≡CBr, CH≡CHO, or CH≡CCF ₃ in presence of O ₂ , at 192 nm. Time-resolved chemiluminescence. IR-Spectro- scopy. P(Ar, or He) = (210-860) mtorr. P(CH≡CH) = (5-25) mtorr. P(O ₂) = (80-500) mtorr.						
CH≡C + H₂ → CH≡CH + H						
Ethyne + Hydrogen molecule						
74 YAM/LAV	DE	1063-1233	6.02(12)	0	3271	2
k ₁ = k ₋₁ K.						
75 LAN/WAG	EX	320	≈1.0(11)			2
Discharge-flow. Mass-spectrometry. P = 4.2 torr.						
79 LAU/BAS	EX	298	4.9(-3)			2
Vacuum-UV flash-photolysis. Kinetic-spectroscopy. Gas-chromatography. k _{ref} : CH≡CH + CH≡C → H + CH≡CC≡CH						
80 TAN/GAR2	ES	625-3400	3.39(13)	0	0	2
CH≡CH Pyrolysis. Based on a modelling study.						
81 KOI/MOR1	ES	1800-2600	2.51(12)	0	0	2
CH≡CH Pyrolysis behind incident shock-waves. P = 380 torr. Based on a modelling study.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 OKA CH=CH/H ₂ photolysis at 147 nm. P(CH=CH) = (0.1-10) torr.	EX	298	(7.75±0.68)(-3)			2	
81 REN/SO CH=C produced by laser photolysis of CH=CH, CH=CBr, or CH=CCHO in presence of O ₂ , at 193 nm. Time-Resolved Chemiluminescence. P(Ar, or He) = (180-400) mtorr. P(O ₂) = (20-400) mtorr.	EX	300	(7.23±1.81)(12)			2	
CH=C + CH ₄ → CH=CH + CH ₃							
Ethyne + Methane							
73 CUL/HUC ¹⁾	RL	298	(1.6±0.5)(-2)			2/2	
73 CUL/HUC ¹⁾	RL	478	1.1(-1)			2/2	
73 CUL/HUC ¹⁾	RL	298-478	(2.36±1.09)	0	1508±153	2/2	
Calculated from the reported reverse ratio.							
¹⁾ k _{ref} : CH=C + CH=CBr → CH=CC=CH + Br							
81 LAU Flash-photolysis. Kinetic-spectroscopy. k independent of He over the (20-700) torr. P-range.	EX	297	(7.23±1.20)(11)			2	
81 OKA Photolysis of CH=CH/CH ₄ mixtures at 147 nm. P(CH=CH) = (0.1-10) torr. k _{ref} : CH=CH + CH=H → CH=CC=CH + H	RL	298	(3.20±0.18)(-2)			2/2	
81 REN/SO CH=C produced by laser photolysis of CH=CH, CH=CBr, or CH=CCHO in presence of O ₂ , at 193 nm. Time-resolved Chemiluminescence. P(Ar, He) = (180-400) mtorr. P(O ₂) = (20-400) mtorr.	EX	300	(2.89±0.60)(12)			2	
CH=C + CH=CH → CH=CC=CH + H							
Ethyne + Ethyne							
73 CUL/HUC	ES	298	1.0(11)	0	1504	2	
75 LAN/WAG Discharge-flow. Mass-spectrometry. P = 4.1 torr.	EX	320	≈3.0(13)			2	
79 LAU/BAS Vacuum-UV flash-photolysis. Kinetic Spectroscopy.	EX	298	(1.87±0.12)(13)			2	
80 FRA/JUS Pyrolysis of CH=CH and CH=CC=CH in Ar, behind shock-waves. Data-fit based on a proposed mechanism. Total Conc. = (0.4-1.6)×10 ¹⁹ molec.cm ⁻³ .	ES	2300-2700	(3.5±0.5)(13)	0	0	2	

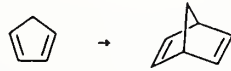
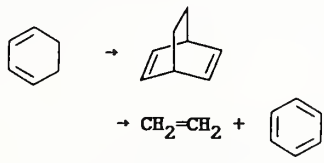
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}\equiv\text{C} + \text{CD}\equiv\text{CD} \rightarrow \text{CH}\equiv\text{CC}\equiv\text{CD} + \text{D}$						
Ethyne + Ethyne- d_2						
73 CUL/HUC $k_{\text{ref}}: \text{CH}\equiv\text{C} + \text{CD}\equiv\text{CD} \rightarrow \text{CH}\equiv\text{CD} + \text{CD}\equiv\text{C}$	RL	298	(2.8 ± 2.5)			2/2
73 CUL/HUC Calculated from the reported reverse ratio. $k_{\text{ref}}: \text{CH}\equiv\text{C} + \text{CH}\equiv\text{CBr} \rightarrow \text{CH}\equiv\text{CC}\equiv\text{CH} + \text{Br}$	RL	298	(6.7 ± 1.6)(-1)			2/2
$\text{CH}\equiv\text{C} + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}\equiv\text{CH} + \text{CH}_3\text{CH}_2$						
Ethyne + Ethane						
73 CUL/HUC $k_{\text{ref}}: \text{CH}\equiv\text{C} + \text{CH}\equiv\text{CBr} \rightarrow \text{CH}\equiv\text{CC}\equiv\text{CH} + \text{Br}$	RL	298	(5.4 ± 0.4)(-1)			2/2
81 LAU Flash-photolysis. Kinetic-spectroscopy. k independent of He over the (20-700) torr. P-range.	EX	297	(3.91 ± 0.24)(12)			2
$\text{CH}\equiv\text{C} + \text{CD}_3\text{CD}_3 \rightarrow \text{CH}\equiv\text{CD} + \text{CD}_3\text{CD}_2$						
Ethyne + Ethane- d_6						
81 LAU Flash-photolysis. Kinetic-spectroscopy. k independent of He over the (20-700) torr. P-range.	EX	297	(1.87 ± 0.30)(12)			2
$\text{CH}\equiv\text{C} + \text{CH}_3\text{C}\equiv\text{CH} \rightarrow \text{CH}\equiv\text{CH} + \text{CH}_2\text{C}\equiv\text{CH}$ (a) $\rightarrow \text{CH}\equiv\text{CC}\equiv\text{CH} + \text{CH}_3$ (b) $\rightarrow \text{CH}\equiv\text{CC}\equiv\text{CCH}_3 + \text{H}$ (c)						
Ethyne + 1-Propyne						
73 CUL/HUC k_a/k_c .	RL	298	(2.5 ± 0.3)(1)			2/2
73 CUL/HUC k_b/k_c .	RL	298	(9.9 ± 1.0)			2/2
73 CUL/HUC 1) $k_{\text{ref}}: \text{CH}\equiv\text{C} + \text{CH}\equiv\text{CBr} \rightarrow \text{CH}\equiv\text{CC}\equiv\text{CH} + \text{C}\equiv\text{CBr}$	RL	298	(4.43 ± 0.58)(-2)			2/2
73 CUL/HUC 1) $k_{\text{ref}}: \text{CH}\equiv\text{C} + \text{CH}\equiv\text{CBr} \rightarrow \text{CH}\equiv\text{CC}\equiv\text{CH} + \text{Br}$	RL	298	(2.38 ± 0.95)(-1)			2/2
1) k_c/k_{ref} . Calculated from the reverse ratio.						
$\text{CH}\equiv\text{C} + \text{CH}\equiv\text{CC}\equiv\text{CH} \rightarrow \text{CH}\equiv\text{CH} + \text{CH}\equiv\text{CC}\equiv\text{C}$ (a) $\rightarrow \text{CH}\equiv\text{CC}\equiv\text{CC}\equiv\text{CH} + \text{H}$ (b)						
Ethyne + 1,3-Butadiyne						
73 CUL/HUC k_a/k_b .	RL	298	(1.1 ± 0.2)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
73 CUL/HUC k_b/k_{ref} . Calculated from the reverse ratio. k_{ref} : $CH\equiv C + CH\equiv CBr \rightarrow CH\equiv CH + C\equiv CBr$	RL	298	(1.71±0.29)			2/2
80 FRA/JUS k_b . $CH\equiv CH$ and $CH\equiv CC\equiv CH$ Pyrolysis in Ar behind shock-waves. Data-fit on the basis of a given mechanism. Total Conc. = (0.4-1.6)×10 ¹⁹ molec.cm ⁻³ .	ES	2400-2700	(2.5±1.5)(13)	0	0	2
$CH\equiv C + CH_2=CHC\equiv CH \rightarrow CH\equiv CH + CH=CHC\equiv CH$						
Ethyne + 1-Buten-3-yne						
80 TAN/GAR2 $CH\equiv CH$ Pyrolysis. Based on modelling study.	ES	625-3400	3.98(13)	0	0	2
$CH\equiv C + (CH_3)_4C \rightarrow CH\equiv CH + (CH_3)_3CCH_3$						
Ethyne + Propane, 2,2-dimethyl-						
73 CUL/HUC k_{ref} : $CH\equiv C + CH\equiv CBr \rightarrow CH\equiv CC\equiv CH + Br$	RL	298	(9.1±0.4)(-1)			2/2
$CH\equiv CH (+ M) \rightarrow CH\equiv C + H (+ M) \quad (a)$ $\rightarrow C + C + H_2 (+ M) \quad (b)$						
Ethyne						
74 ALT k_a .	EX	1700-2000	1.0(15)	0	55360	1
78 CUN/FUS $k_{overall}$. M = Ar. Incident shock-waves. P = (1-2) bar.	ES	1500-2000	1.58(7)	0	24899	1
75 BEC/MAC ¹⁾ k_a . M = Ar.	DE	4860-6920	6.02(15)	0	75419	2
75 BEC/MAC ¹⁾ k_a . M = H.	DE	4860-6920	5.42(13)	0	12028	2
¹⁾ $CH\equiv CH$ Shock-wave pyrolysis in Ar. Best-fit of experimental data.						
80 FRA/JUS k_a . M = Ar. $CH\equiv CH$ and $CH\equiv CC\equiv CH$ pyrolysis in Ar, behind shock-waves. Total Conc. = (0.4-1.6)×10 ¹⁹ molec.cm ⁻³ .	EX	2100-3000	(3.6±0.6)(16)	0	53600±400	2
82 THR/WIN k_b . M = Ar. $CH\equiv CH$ decomposition in an Ar plasma. Mass-spectrometry.	EX	3900-4250	1.00(14)	0	30673±8420	2 10.0

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}\equiv\text{CH} + \text{CH}\equiv\text{CH} \rightarrow \text{CH}\equiv\text{CCH}=\text{CH} + \text{H}$ (a) $\rightarrow \text{CH}\equiv\text{CC}\equiv\text{CH} + \text{H} + \text{H}$ (b) $\rightarrow \text{CH}_2=\text{CHC}\equiv\text{CH}$ (c)							
Ethyne							
80 TAN/GAR2 k_a . $\text{CH}\equiv\text{CH}$ pyrolysis. Modelling study.	ES	625-3400	2.00(12)	0	23095	2	
80 BAR/DOV ¹⁾ k_a .	EX	2650	1.98(10)			2	
80 BAR/DOV ¹⁾ k_a . Based on present and previous k's.	SE	1600-2650	6.0(13)	0	20634	2	
¹⁾ $\text{CH}\equiv\text{CH}$ pyrolysis behind shock-waves.							
80 FRA/JUS ²⁾ k_a .	ES	1845-2000	(1.51±0.79)(8)	0	0	2	
80 FRA/JUS ²⁾ k_b .	ES	1845-2000	(3.0±1.0)(8)	0	0	2	
²⁾ $\text{CH}\equiv\text{CH}/\text{CH}\equiv\text{CC}\equiv\text{CH}$ Pyrolysis in Ar behind shock-waves. Data-fit based on a proposed mechanism. Total Conc. = (0.4-1.6)×10 ¹⁹ molec.cm ⁻³ .							
77 OGU1 ³⁾	EX	1000-1670	2.45(14)	0	23352±705	2	1.82
77 OGU2 ³⁾	EX	1000-1600	(1.48±0.18)(14)	0	22245±755	2	
³⁾ k_c .							
$\text{CH}\equiv\text{CH} + $ 							
Ethyne + 1,3-Cyclopentadiene							
$\rightarrow$ Bicyclo[2.2.1]hepta-2,5-diene (2,5-Norbornadiene)							
75 WAL/WEL Static system. Gas-chromatography. Diels-Alder addition of $\text{CH}\equiv\text{CH}$ to 1,3-Cyclopentadiene.	EX	525-756	3.24(7)	0	12174±75	2	1.12
$\text{CH}\equiv\text{CH} + $ 							
Ethyne + 1,3-Cyclohexadiene							
$\rightarrow$ Bicyclo[2.2.2]octa-2,5-diene $\rightarrow$ Ethene + Benzene							
82 HUY/LEE Thermal Diels-Alder addition of $\text{CH}\equiv\text{CH}$ to 1,3-Cyclohexadiene. NMR-Spectrometry. Gas-chromatography. Static system. P(1,3-Cyclohexadiene) = (8-62) torr. P($\text{CH}\equiv\text{CH}$) = (25-112) torr.	EX	450-592	3.09(10)	0	13664±60	2	1.12

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2=\text{CH} (+\text{M}) \rightarrow \text{CH}=\text{CH} + \text{H} (+\text{M})$						
Ethenyl						
73 PEE/MAH2	ES	1500	2.0(12)			2
$\text{CH}_2=\text{CH} + \text{CH}=\text{CH} \rightarrow \text{CH}_2=\text{CHC}=\text{CH} + \text{H}$						
Ethenyl + Ethyne						
80 TAN/GAR2	ES	625-3400	1.58(13)	0	12630	2
CH=CH Pyrolysis. Based on a modelling study.						
$\text{CH}_2=\text{CH} + \text{CH}_2=\text{CH} \rightarrow \text{CH}=\text{CH} + \text{CH}_2=\text{CH}_2$ (a)						
$\rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2$ (b)						
Ethenyl						
75 IBU/TAK	RL	296	8.7(-2)			2/2
k_a/k_b . Conventional vacuum system.						
$\text{CH}_2=\text{CH} + \text{CH}_3\text{CH}_2 \rightarrow \text{CH}=\text{CH} + \text{CH}_3\text{CH}_3$ (a)						
$\rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{CH}_2$ (b)						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2$ (c)						
Ethenyl + Ethyl						
75 IBU/TAK ¹⁾	RL	296	3.69(-1)			2/2
k_a/k_c .						
75 IBU/TAK ¹⁾	RL	296	6.8(-1)			2/2
k_b/k_c .						
¹⁾ Conventional vacuum system.						
$\text{CH}_2=\text{CH}_2 (+\text{M}) \rightarrow \text{CH}_2=\text{CH} + \text{H} (+\text{M})$ (a)						
$\rightarrow \text{CH}=\text{CH} + \text{H}_2 (+\text{M})$ (b)						
Ethene						
73 ROT/JUS ¹⁾	EX	1675-2210	1.78(17)	0	39004	2
77 JUS/ROT ¹⁾	EX	1700-2200	(3.8±1.3)(17)	0	49400±900	2
80 TAN/GAR1 ¹⁾	EX	2000-2450	3.09(17)	0	48114	2
Pyrolysis behind incident shock-waves.						
Total Conc. = (1.1-2.2)×10 ¹⁸ molec. ⁻³ .						
¹⁾ k_a . M = Ar.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_2=\text{CH} + \text{CH}_3\text{CH}_2$ (a)							
$\rightarrow \square$ (b)							
Ethene							
81 AYR/BAC k_a . Static system pyrolysis. Gas-chromatography. k determined relative to the reaction: $\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3 + \text{CH}_2\text{CH}=\text{CH}_2$	RN	750	1.58(16)	0	33719	2	
72 QUI/KNE k_b .	EX	723-786	6.92(10)	0	22043	2	1.15
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$							
Ethene + 1-Propene							
78 RIC/BAC Static system pyrolysis. P(olefin) = (33-300) torr.	EX	682-754	2.82(10)	0	18621±503	2	2.0
$\text{CH}_2=\text{CH}_2 + \text{cis-CH}_3\text{CH}=\text{CHCH}_3$							
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2$ (a)							
$\rightarrow \text{cis-CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2$ (b)							
Ethene + 2-Butene, (Z)-							
78 RIC/SCA k_a . Static system pyrolysis. P(olefin) = (20-200) torr.	EX	689-754	1.12(10)	0	18369±503	2	2.0
77 SCA/BAC k_b . A-factor recalculated from the reported experimental data. Average k.	EX	663-703	(1.28±0.16)(12)	0	24270±71	2	
77 SCA/RIC k_b . Determined from present and literature data for the rate of geometric isomerization of 1,2- Dimethyl-cyclobutane. Static system. P = 12 atm.	RN	693	8.0(-4)			2	
$\text{CH}_2=\text{CH}_2 + \text{trans-CH}_3\text{CH}=\text{CHCH}_3$							
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2$ (a)							
$\rightarrow \text{trans-CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2$ (b)							
Ethene + 2-Butene, (E)-							
78 RIC/SCA k_a . Static system pyrolysis. P(olefin) = (20-200) torr.	EX	689-754	3.55(10)	0	18621±503	2	2.0
77 SCA/BAC k_b . A-factor recalculated from the reported experimental data.	EX	663-703	(4.49±0.89)(11)	0	23136±120	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
77 SCA/BAC k_b/k_{ref} . Average, estimated ratio. k_{ref} : $CH_2=CH_2 + cis-CH_3CH=CHCH_3$ $\rightarrow cis-CH_3CHCH(CH_3)CH_2CH_2$	RL	663-703	(1.80±0.10)	0	0	2/2
77 SCA/RIC ¹⁾ k_b/k_{ref} . k_{ref} : $CH_2=CH_2 + cis-CH_3CH=CHCH_3$ $\rightarrow cis-CH(CH_3)CH(CH_3)CH_2CH_2$	RL	693	(1.86±0.1)			2/2
77 SCA/RIC ¹⁾ k_b . Determined from present and literature data for the rate of geometric isomerization of 1,2-Dimethyl-cyclobutane. ¹⁾ Static system. P = 12 atm.	RN	693	1.48(-3)			2
$CH_2=CH_2 + (CH_3)_2C=CH_2 \rightarrow CH_3CH_2C(CH_3)=CH_2$ Ethene + 1-Propene, 2-methyl-						
78 RIC/BAC Pyrolysis in a static system. P(olefin) = (33-300) torr.	EX	682-754	1.78(11)	0	19124±503	2 2.0
$CH_2=CH_2 + $  $\rightarrow $ 						
Ethene + 1,3-Cyclopentadiene $\rightarrow$ Bicyclo(2.2.1)hept-2-ene (Norbornene)						
76 WAL/WEL Diels-Alder addition of Ethene to 1,3-Cyclopentadiene in a static system. Gas-chromatography.	EX	521-570	3.89(10)	0	11912±785	2 4.27
$CH_2=CH_2 + CH_2=C(CH_3)CH=CH_2 \rightarrow $ 						
Ethene + 1,3-Butadiene, 2-methyl- $\rightarrow$ Cyclohexene, 1-methyl-						
78 SIM Single-pulse shock-tube. From k_p and thermodynamic data.	DE	1000-1180	1.32(11)	0	14900	1
$CH_2=CH_2 + $  $\rightarrow CH_3CH_3 + $ 						
Ethene + Cyclopentene $\rightarrow$ Ethane + 1,3-Cyclopentadiene						
80 LAL/BAC Static system. P(Total) = (150-350) torr.	EX	598-778	1.0(15)	0	25013	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_2=\text{CH}_2 + $  $ \rightarrow $ 							
Ethene + 1,3-Cyclohexadiene $\rightarrow$ Bicyclo[2.2.2]oct-2-ene							
80 HUY/RIG Vacuum system. Gas-chromatography. Diels-Alder addition of Ethene to 1,3-Cyclohexadiene.	EX	466-591	4.57(9)	0	13070 $\pm$ 25	2	1.05
77 TAN k_b . M = Ar. Pyrolysis in shock-waves. Laser-schlieren. P = (0.9-1.7) kPa. of Ethene in Ar.	EX	2000-2500	1.2(17)	0	38700	2	
77 JUS/ROT k_b . M = Ar.	EX	1700-2200	(2.6 $\pm$ 0.5)(17)	0	39900 $\pm$ 500	2	
80 TAN/GAR1 k_b . M = Ar. Ethene pyrolysis. Incident shock-waves. Total Conc. = (1.1-2.2) $\times 10^{18}$ molec.cm $^{-3}$.	EX	2000-2450	2.95(17)	0	40897	2	
78 CUN/FUS k_{overall} . M = Ar. Incident shock-waves. P = (1-2) bar.	ES	1500-2000	6.31(6)	0	27305	1	
$\text{CH}_3\text{CH}_2 (+\text{M}) \rightarrow \text{CH}_2=\text{CH}_2 + \text{H} (+\text{M})$							
Ethyl							
79 PRA/ROG1 M = Ar. Ethane pyrolysis in a wall-less reactor. P(Ar) = 600 torr. Gas-chromatography. Data-fit.	CO	941-1073	3.16(13)	0	21050 $\pm$ 1443	1	5.01
81 COR/MAR Ethane pyrolysis. Flow-reactor. Based on a proposed mechanism. P = 40 torr.	ES	803	2.0(2)			1	
76 CHE/BAC	CO	995	3.29(4)			2	
80 PAC/WIM2 Estimated k. Ethane pyrolysis. Flow-reactor. Gas-chromatography. P = 100 torr.	RN	903	(3.6 $\pm$ 0.5)(3)			2	
$\text{CH}_3\text{CH}_2 + \text{O}_2 \rightarrow \text{CH}_2=\text{CH}_2 + \text{HO}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{O}_2$ (b) $\rightarrow \text{CH}_3\text{CHO} + \text{OH}$ (c) $\rightarrow $  $ + \text{OH}$ (d)							
Ethyl + Oxygen molecule							
71 BAL/LAN k_a/k_{ref} . Estimated ratio. k_{ref} : $\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CHO} \rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CO}$	RL	713	(4.1 $\pm$ 0.5)(1)			2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
71 BAK/BAL ¹⁾	ES	896	1.0(11)				2
71 BAL/LAN ¹⁾	ES	713	8.2(10)				2
80 BAL/PIC ¹⁾ Static system. Gas-chromatography.	EX	673-813	8.51(11)	0	1949		2
81 PLU/RVA2 ¹⁾ ²⁾ M = He. k is independent of [He].	EX	295	(1.26±0.30)(11)				2
¹⁾ k _a .							
81 PLU/RVA2 ²⁾ k _b . M = He. k strongly dependent on [He]. Limiting high-pressure k.	ES	295	~2.65(12)				2
71 BAK/BAL k _c .	ES	773	3.4(8)				2
71 BAK/BAL k _d .	ES	773	2.6(9)				2
81 PLU/RVA2 ²⁾ k _{overall} . M = He. [He] = 2.0x10 ¹⁶ molec.cm ⁻³ . k increases with [He].	EX	295	(7.23±1.80)(11)				2
81 PLU/RVA2 ²⁾ k _{overall} . M = He. [He] = 3.4x10 ¹⁷ molec.cm ⁻³ . k increases with [He].	EX	295	(2.17±0.54)(12)				2
²⁾ Flow-reactor. Mass-spectrometry. CH ₃ CH ₂ produced by reaction of Cl with Ethane.							
CH₃CH₂ + O₃ → products							
Ethyl + Ozone							
82 PAL Photoionization Mass-spectrometry. CH ₃ CH ₂ generated by photodissociation of CH ₃ CH ₂ NO ₂ . P = 2 torr.	EX	298	(1.40±0.22)(13)				2
CH₃CH₂ + H₂ → CH₃CH₃ + H							
Ethyl + Hydrogen molecule							
71 BAL/LAN k _{ref} : CH ₃ CH ₂ + CH ₃ CH ₂ CHO → CH ₃ CH ₃ CH ₃ CH ₂ CO Estimated ratio.	RL	713	(1.24±0.17)(-1)				2/2
71 BAL/LAN	ES	713	2.15(8)				2
82 CAO/BAC Cylindrical quartz reactor, with packed or unpacked vessels. Static system. CH ₃ CH ₂ generated by reacting Ethene with H ₂ . [CH ₂ =CH ₂] = 4.6x10 ¹⁴ molec.cm ⁻³ . P(Total) = (100-300) torr.	EX	1111-1200	3.98(13)	0	11575		2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃CH₂ + D₂ → CH₃CH₂D + D						
Ethyl + Deuterium molecule						
71 BAL/LAN	ES	713	(4.76±0.50)(-2)			2/2
k _{ref} : CH ₃ CH ₂ + CH ₃ CH ₂ CHO → CH ₃ CH ₃ CH ₃ CH ₂ CO						
71 BAL/LAN	ES	713	8.3(7)			2
CH₃CH₂ + NO → CH₃CH₂NO						
Ethyl + Nitrogen oxide (NO)						
74 PRA/VEL	EX	295	(1.2±0.1)(11)			2
76 PRA/VEL2	EX	325-521	(1.4±0.2)(11)	0	0	2
CH₃CH₂ + CO → CH₃CH₂CO						
Ethyl + Carbon monoxide						
73 WAT/THO	RN	238-378	1.55(11)	0	2416±50	2
CH₃CH₂ + CH₄ → CH₃CH₃ + CH₃						
Ethyl + Methane						
76 CHE/BAC	CO	995	9.0(7)			2
CH₃CH₂ + CH₃CH₂ → CH₂=CH₂ + CH₃CH₃ (a)						
→ CH ₃ CH ₂ CH ₂ CH ₃ (b)						
Ethyl						
71 FAL/SUN ¹⁾	RL	298	1.4(-1)			2/2
73 HAR/TAN ¹⁾	RL	298	(1.6±0.4)(-1)			2/2
CH ₂ =CH ₂ photolysis at 163.4 nm.						
73 HAR/TAN ¹⁾	RL	298	(2.1±0.6)(-1)			2/2
CH ₂ =CH ₂ photolysis at 184.9 nm.						
75 HOO/SIM ¹⁾	RL	173-298	1.45(-1)			2/2
77 MAR/MAC ¹⁾	RL	553-673	(1.4±0.3)(-1)			2/2
Thermolysis in a vacuum system.						
79 ADA/BAS3 ¹⁾	RL	298	(1.39±0.13)(-1)			2/2
Flash-photolysis. Absorption-spectroscopy.						
¹⁾ k _a /k _b .						
72 TEN/JON ²⁾	CO	303-603	7.59(12)	0	96	2
Data-fit to a proposed mechanism.						
72 HIA/BEN2 ²⁾	ES	350-410	3.98(11)	0	0±101	2
72 MAR/PUR ²⁾	ES	350-950	2.51(11)	0	0	2
72 PAC/PUR1 ²⁾	DE	951	3.16(11)			2
75 HUG/MAR ²⁾	ES	693-803	2.51(11)	0	0	2
76 GOL/CHO ²⁾	EX	860	4.5(12)			2
Low-pressure k.						
76 PAR/QUI ²⁾	RN	298	(7.83±1.81)(12)			2

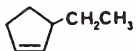
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 ADA/BAS3 ²) Flash-photolysis. Absorption-spectroscopy.	RN	298	(1.24±0.23)(13)			2
80 PAC/WIM2 ²) Ethane pyrolysis in a flow-reactor. Gas-chromatography. P = 100 torr.	ES	903	(1.1±0.4)(13)			2
2) k _b .						
79 ADA/BAS3 k _a + k _b . Flash-photolysis. Absorption spectroscopy.	EX	298	(1.40±0.27)(13)			2
81 COR/MAR k _a + k _b . Ethane pyrolysis in a continuous- flow stirred reactor. Gas-chromatography. P = 40 torr.	EX	803	5.6(12)			2
82 DEM/LES k _a + k _b . Flash-photolysis. Laser Resonance- absorption. CH ₃ CH ₂ generated by flashing NH ₃ in presence of Ethene. Best-fit by simulation.	DE	298	1.2(13)			2
CH₃CH₂ + CH₃CHO → CH₃CH₂CH(O·)CH₃						
Ethyl + Acetaldehyde						
75 BAT/MCC	ES	393-473	7.94(11)	0	0±503	2
CH₃CH₂ + CH₃CH₂NO → (CH₃CH₂)₂NO						
Ethyl + Ethane, nitroso-						
72 TAN/LAM Lower-limit k.	EX	329	≥1.45(10)			2
CH₃CH₂ + CH₃CH₂CHO → CH₃CH₃ + CH₃CH₂CO						
Ethyl + Propanal						
71 BAL/LAN k _{ref} : CH ₃ CH ₂ + H ₂ → CH ₃ CH ₃ + H	RL	713	(8.1±1.0)			2/2
71 BAL/LAN k _{ref} : CH ₃ CH ₂ + D ₂ → CH ₃ CH ₂ D + D	RL	713	(2.1±0.2)(1)			2/2
CH₃CH₂ + CH₂=CHCH₂CH₂ → CH₂=CH₂ + CH₂=CHCH₂CH₃ (a)						
→ CH ₃ CH ₃ + CH ₂ =CHCH=CH ₂ (b)						
→ CH ₂ =CHCH ₂ CH ₂ CH ₂ CH ₃ (c)						
Ethyl + 3-Butenyl						
75 STE/RAB (k _a + k _b)/k _c . Dispr./Comb. ratio.	RL	298	(3.0±0.6)(-1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{CH}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)_2$ Ethyl + 1-Propene, 2-methyl-							
78 MYS/SO $\text{CH}_3\text{CH}_2\text{BR}$ ^{60}Co γ -irradiation. Gas-chromatography.	EX	323-423	(1.26±0.04)(5)	0	805±50	2	
$\text{CH}_3\text{CH}_2 + \square^* \rightarrow \text{CH}_2=\text{CH}_2 + \square$ (a)							
$\rightarrow \text{CH}_3\text{CH}_3 + \square$ (b)							
$\rightarrow \square\text{CH}_2\text{CH}_3$ (c)							
Ethyl + Cyclobutyl							
75 STE/RAB ($k_a + k_b$)/ k_c . Dispr./Comb. ratio.	RL	298	(2.3±0.2)(-1)			2/2	
$\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CHCH}_3$ (b)							
Ethyl + Butane							
72 PAC/PUR1 ¹⁾	ES	869-952	3.16(13)	0	10116±856	2	2.51
74 HUG/MAR ¹⁾ Calculation based on experimental data.	DE	895-981	7.94(13)	0	11162±806	2	2.51
76 YAM/NAM ¹⁾ ¹⁾ $k_a + k_b$.	EX	980-1060	3.16(12)	0	6442±1359	2	3.55
$\text{CH}_3\text{CH}_2 + \text{CH}_3\text{C}(\text{O})\text{C}(\text{O})\text{CH}_3 \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_3$ (a) $\rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_2\text{C}(\text{O})\text{C}(\text{O})\text{CH}_3$ (b) $\rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_3 + \text{CH}_3\text{CO}$ (c)							
Ethyl + 2,3-Butanedione (Biacetyl)							
76 SCH/KNO k_a .	RN	525-556	2.51(8)	0	3573±302	2	2.0
76 SCH/KNO k_b .	RN	525-556	3.98(12)	0	5385±1560	2	15.8
76 SCH/KNO k_c .	RN	525-556	3.98(8)	0	2969±302	2	2.0
$\text{CH}_3\text{CH}_2 + (\text{CH}_3\text{CH}_2)_2\text{O} \rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$ Ethyl + Ethane, 1,1'-oxybis- (Diethyl ether)							
77 SER/LAB Diethyl ether/Acetaldehyde pyrolysis. k determined on the basis of a proposed mechanism.	ES	763-823	3.0(11)	0	4026	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}_2 + (\text{CH}_3\text{CH}_2)_2\text{S} \rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3\text{CHSCH}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_2\text{CH}_2\text{SCH}_2\text{CH}_3$ (b) Ethyl + Ethane, 1,1'-thiobis- (Diethyl sulfide)	RN	298-461	(7.4±0.5)(13)	0	3452±49	2
81 EKW/SAF2 k_a . H atoms generated by Hg-photosensitized decomposition of H_2 . Vacuum system. k determined relative to the reaction: $\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{H}_2\text{CH}_3$ P(Diethyldisulfide) = (1-32) torr. P(H_2) ~ 580 torr.						
$\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_2\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_3$ Ethyl + Diazene, diethyl-	RN	525-556	7.94(11)	0	3775±1359	2 10.0
76 SCH/KNO $\text{CH}_3\text{CH}_2 + (\text{CH}_3\text{CH}_2)_2\text{NOH} \rightarrow \text{CH}_3\text{CH}_3 + (\text{CH}_3\text{CH}_2)_2\text{NO}$ Ethyl + Ethanamine, N-ethyl-N-hydroxy-	RN	298	(3.0±0.7)(9)			2
78 ABU/ENC Azoethane photolysis. The abstract gives a rate constant of: $7.2 \times 10^8 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, smaller by a factor of 4.4 than the above tabulated k value, which was reported in the text. k determined relative to the reaction: $\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$. It probably involves abstraction from the hydroxylic Hydrogen.						
$\text{CH}_3\text{CH}_2 + $  $\rightarrow \text{CH}_2=\text{CH}_2 + $  (a) $\rightarrow \text{CH}_3\text{CH}_3 + $  (b) $\rightarrow $  (c)						
Ethyl + 2-Cyclopenten-1-yl 75 STE/RAB $(k_a + k_b)/k_c$. Dispr./Comb. ratio.	RL	298	(1.6±0.3)(-1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃CH₂ + CH₃CH=CHCH₂CH₂						
→ CH ₃ CH ₃ + cis-CH ₃ CH=CHCH=CH ₂ (a)						
→ CH ₃ CH ₃ + trans-CH ₃ CH=CHCH=CH ₂ (b)						
→ CH ₂ =CH ₂ + cis-CH ₃ CH=CHCH ₂ CH ₃ (c)						
→ CH ₂ =CH ₂ + trans-CH ₃ CH=CHCH ₂ CH ₃ (d)						
→ CH ₃ CH=CHCH ₂ CH ₂ CH ₂ CH ₃ (e)						
Ethyl + 3-Pentenyl						
75 STE/RAB ¹⁾ (k _a + k _b)/k _e .	RL	298	(8.7±1.0)(-2)			2/2
75 STE/RAB ¹⁾ (k _c + k _d)/k _e .	RL	298	(9.3±0.3)(-2)			2/2
¹⁾ Dispr./Comb. ratios.						
CH₃CH₂ + 						
→ CH ₂ =CH ₂ +  (a)						
→ CH ₃ CH ₃ +  (b)						
→  (c)						
Ethyl + Cyclopentyl						
75 STE/RAB (k _a + k _b)/k _c . Dispr./Comb. ratio.	RL	298	(2.6±0.3)(-1)			2/2
CH₃CH₂ + CH₃C(O)C(O)CH₂CH₃						
→ CH ₃ CH ₃ + CH ₂ C(O)C(O)CH ₂ CH ₃ (a)						
→ CH ₃ CH ₃ + CH ₃ C(O)C(O)CHCH ₃ (b)						
→ CH ₃ CH ₃ + CH ₃ C(O)C(O)CH ₂ CH ₂ (c)						
→ (CH ₃ CH ₂) ₂ CO + CH ₃ CO (d)						
Ethyl + 2,3-Pentanedione						
74 SCH/KNO k _b /k _a . T-dependence not detectable.	RL	362-398	≈4.5	0	0	2/2
74 SCH/KNO k _c /k _a . T-dependence not detectable.	RL	362-398	≈3.0(-1)	0	0	2/2
74 SCH/KNO (k _a + k _b + k _c)/k _d .	RL	362-398	5.01(1)	0	1409±1158	2/2 6.31

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}_2 + $  $\rightarrow \text{CH}_2=\text{CH}_2 + $  (a)						
$\rightarrow \text{CH}_3\text{CH}_3 + $  (b)						
$\rightarrow $  (c)						
Ethyl + Cyclohexyl						
75 STE/RAB	RL	298	$\leq (3.4 \pm 0.5)(-1)$			2/2
$(k_a + k_b)/k_c$.						
Dispr./comb. ratio.						
$\text{CH}_3\text{CH}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}_3$						
$\rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3(\text{CH}_2)_4\text{CH}_2$ (a)						
$\rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3(\text{CH}_2)_3\text{CHCH}_3$ (b)						
$\rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3(\text{CH}_2)_2\text{CHCH}_2\text{CH}_3$ (c)						
Ethyl + Hexane						
76 YAM	RN	973-1088	1.8(13)	0	8052	2
$k_a + k_b + k_c$.						
$\text{CH}_3\text{CH}_3 (+\text{M}) \rightarrow \text{CH}_3 + \text{CH}_3 (+\text{M})$ (a)						
$\rightarrow \text{CH}_2=\text{CH}_2 + \text{H}_2 (+\text{M})$ (b)						
Ethane						
72 PAC/PUR2	EX	920-1040	5.01(16)	0	44505	1
k_a .						
73 BUR/SKI	CO	1000-1500	7.94(16)	0	45043	1
k_a . M = Ar. Limiting high-pressure k.						
RRKM Correlation of experimental data.						
76 CLA/QUI	EX	778-878	1.17(16)	0	43533±252	1 1.38
k_a .						
79 OLS/GAR ¹⁾	CO	1330-2500	7.07(16)	0	45361	1
Extrapolated limiting high-pressure expression						
obtained by applying RRK or RRKM methods to						
the experimental Ethane pyrolysis data from						
79 OLS/TAN.						
79 OLS/GAR ¹⁾	CO	250-2500	2.04(16)	0	44210	1
Limiting high-pressure k, extended to lower						
T-range by combining k's for CH_3 recombination						
at low T, with k's for Ethane decomposition.						
¹⁾ k_a . M = Ar. Decomposition of Ethane behind						
incident shock-waves by Laser-absorption and						
Laser-schlieren experiments.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
79 ROT/JUS2 a. Shock-tube. Atomic resonance-absorption. k determined by computer simulation. Total Conc. = (0.2-2.3) × 10 ¹⁹ molec.cm ⁻³ .	DE	1450-2100	2.0(15)	0	42000	1	
79 TRE k _a . Thermolysis. P = (3-700) torr.	EX	840-913	5.25(16)	0	44716 ± 342	1	1.48
80 BHA/FRA k _a . Shock-tube. Resonance-absorption. Computer simulation based on a proposed mechanism.	DE	1700-2300	8.0(12)	0	35400	1	
80 PAC/WIM2 k _a . Ethane pyrolysis. Flow-reactor. P = 100 torr.	EX	903	(1.15 ± 0.16)(-5)			1	
81 CHI/SKI2 k _a . M = Ar. Ethane pyrolysis behind reflected shock-waves. Resonance-absorption spectroscopy. k determined relative to the reaction: $\text{CH}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2$ P(Total) = (2-3) atm.	RN	1240-1700	2.8(15)	0	42400	1	
81 COR/MAR k _a . Ethane pyrolysis in a continuous-flow stirred tank reactor. Gas-chromatography. P = 40 torr.	EX	840	4.1(-8)			1	
80 BAU/DUX ²⁾ High-pressure k. Critical review.	RE	750-1500	2.40(16)	0	44010 ± 3170	1	3.16
81 BAR ²⁾ Pyrolysis in a quartz reactor.	EX	963-1333	1.55(14)	0	33468	1	
81 BAR ²⁾ Pyrolysis in an inconel reactor.	EX	963-1333	1.0(10)	0	23905 ± 5033	1	
²⁾ k _b .							
71 ILL/WEL ³⁾	EX	993-1097	4.57(15)	0	36633	1	
71 KOR/KAL ³⁾ Pyrolysis in a quartz reactor. Gas-chromatography. P(Total) = 100 torr.	EX	1070-1200	5.0(16)	0	39758	1	1.2
72 ILL/SZA ³⁾	EX	933-1097	6.44(14)	0	34701	1	1.1
74 BAK/NOV ³⁾	EX	973-1123	1.37(16)	0	38853 ± 1510	1	
78 COH ³⁾ Pyrolysis in a flow-reactor.	EX	1040-1190	3.0(16)	0	44288	1	
³⁾ k _{overall} .							
78 VER/BEL ⁴⁾ k _{ref} : CH ₃ CH ₂ CH ₃ → products.	RL	1043-1103	(3.2 ± 0.7)(-1)			1/1	
78 VER/BEL ⁴⁾ k _{ref} : CH ₃ CH ₂ CH ₂ CH ₃ → products.	RL	1023-1193	(1.75 ± 0.15)(-1)			1/1	
⁴⁾ k _{overall} /k _{ref} . Pyrolysis in a flow-reactor.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
71 IZO/KIS k _a . Shock waves. Best data fit. Total conc.: 5x10 ¹⁷ molec.cm ⁻³ .	DE	1400-2200	2.4(21)	0	44288	2	
79 OLS/TAN k _a . M = Ar. Decomposition behind incident shock-waves. Laser-absorption. Laser-schlieren. Computer simulation by fitting the data to an assumed mechanism with 14 steps. The preexponential factor expressed as: A(T/298) ^{-25.26} .	DE	1300-2500	6.34(48)	-25.26	80320	2	
CH₃CH₃[†] → CH₃ + CH₃							
Ethane							
76 SHI/OBI At 163 nm. CH ₃ CH ₃ [†] formed by CH ₂ [†] + CH ₄ .	EX	298	5.0(9)			1	
76 SHI/OBI At 147 nm. CH ₃ CH ₃ [†] formed by CH ₂ [†] + CH ₄ .	EX	298	6.0(9)			1	
78 LIN/YEH Hg-sensitized photolysis. CH ₃ CH ₃ ^{>} formed by H + CH ₃ CH ₂ . P = (1.5-30) torr.	EX	308	1.7(-7)			1	
CD₃CD₃ → CD₃ + CD₃							
Ethane-d ₆							
76 CLA/QUI	EX	778-878	3.20(16)	0	44269±121	1	1.16
81 CHI/SKI2 M = Ar. Pyrolysis behind reflected shock-waves. Resonance-absorption. k determined relative to the reaction: CD ₃ + CD ₃ CD ₃ → CD ₄ + CD ₃ CD ₂ P(Total) = (2-3) atm.	RN	1240-1700	2.8(15)	0	42400	1	
CH=C=O + O₂ → products							
Ethenyl, 2-oxo- + Oxygen molecule							
73 JON/BAY2 k _{ref} : CH=C=O + O → products.	RL	296	(1.8±0.3)(-2)			2/2	
73 JON/BAY2	RN	296	(2.2±1.2)(10)			2	
CH=C=O + CH≡CH → products							
Ethenyl, 2-oxo- + Ethyne							
73 JON/BAY1 Upper-limit k.	EX	298	<5.0(8)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_2=\text{C}=\text{O} + \text{CH}_2=\text{C}=\text{O} \rightarrow$ 							
Ethenone (Ketene)							
72 BLA/DAV	EX	498-596	1.78(8)	0	8901±132	2	
$\text{CH}_2=\text{C}=\text{O} + \text{CH}_3\text{COOH} \rightarrow (\text{CH}_3\text{CO})_2\text{O}$							
Ethenone (Ketene) + Acetic acid							
76 BLA/VAY	EX	368-489	1.26(9)	0	6003±114	2	1.29
76 BLA/VAY	EX	428	1.02(3)			2	
$\text{CH}_2=\text{C}=\text{O} + \text{CH}_3\text{CH}_2\text{COOH} \rightarrow \text{CH}_3\text{CH}_2\text{COOCOCH}_3$							
Ethenone (Ketene) + Propanoic acid							
76 BLA/VAY	EX	368-489	1.74(9)	0	6102±90	2	1.23
76 BLA/VAY	EX	428	1.12(3)			2	
$\text{CH}_2=\text{C}=\text{O} + \text{CH}_3\text{CH}_2\text{CH}_2\text{COOH} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{COOCOCH}_3$							
Ethenone (Ketene) + Butanoic acid							
76 BLA/VAY	EX	428	1.26(3)			2	
$\text{CH}_2=\text{C}=\text{O} + (\text{CH}_3)_2\text{CHCOOH} \rightarrow (\text{CH}_3)_2\text{CHCOOCOCH}_3$							
Ethenone (Ketene) + Propanoic acid, 2-methyl-							
76 BLA/VAY	EX	428	1.57(3)			2	
$\text{CH}_2=\text{C}=\text{O} + (\text{CH}_3)_3\text{CCOOH} \rightarrow (\text{CH}_3)_3\text{CCOOCOCH}_3$							
Ethenone (Ketene) + Propanoic acidm 2,2-dimethyl-							
76 BLA/VAY	EX	368-489	1.55(9)	0	5754±100	2	1.26
76 BLA/VAY	EX	428	2.23(3)			2	
$\text{CH}_2=\text{C}=\text{O} + (\text{CH}_3)_3\text{CCH}_2\text{COOH} \rightarrow (\text{CH}_3)_3\text{CCH}_2\text{COOCOCH}_3$							
Ethenone (Ketene) + Butanoic acid, 3,3-dimethyl-							
76 BLA/VAY	EX	428	1.63(3)			2	
$\text{CH}_3\text{CO} (+ \text{M}) \rightarrow \text{CH}_3 + \text{CO} (+ \text{M})$							
Ethyl, 1-oxo- (Acetyl)							
73 FRE/VIN	RN	326	(1.91±0.3)(1)			1	
Estimated k on the basis of a proposed mechanism.							
74 SZI/WAL ¹⁾	RL	507	(2.41±0.34)(-8)			1/2	
k _{ref} : CH ₃ CO + HI → CH ₃ CHO + I							
74 SZI/WAL ¹⁾	RN	498-525	2.00(13)	0	10970±902	1	3.16
Estimated, limiting high-pressure k.							
¹⁾ M = N ₂ , or cy-(CF ₂) ₄ .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
74 WAT/WOR	RN	333-413	1.58(13)	0	8661±241	1 2.0
82 ANA/MAW ²⁾	EX	323	(2.45±0.74)(1)			1
82 ANA/MAW ²⁾	EX	343	(1.86±0.56)(2)			1
Limiting high-pressure k.						
82 ANA/MAW ²⁾	EX	343	(1.87±0.56)(7)			2
Limiting low-pressure k.						
²⁾ M = CO. Molecular modulation spectroscopy.						
CH ₃ CO produced by Azomethane/CO photolysis.						
[Azomethane] = 1.0x10 ¹⁷ molec.cm ⁻³ .						
[CO] = (0.3-2.7)x10 ¹⁹ molec.cm ⁻³ .						
CH ₃ CO + O ₂ → CH ₃ C(O)O ₂						
Ethyl, 1-oxo- (Acetyl) + Oxygen molecule						
74 DIX/SKI1	ES	336-357	(1.2±0.3)(10)			2
82 MCD/LEN	EX	298	(1.20±0.24)(12)			2
CH ₃ CO generated by Photolysis of Acetone, or Acetyl-Acetone vapor in (1-4) torr. He.						
CH ₃ CO + NO → products						
Ethyl, 1-oxo- (Acetyl) + Nitrogen oxide (NO)						
82 MCD/LEN	EX	298	(5.60±1.63)(11)			2
CH ₃ CO generated by Photolysis of Acetone, or Acetylacetone vapor, in (1-4) Torr He.						
CH ₃ CO + NO ₂ → CH ₃ CO ₂ + NO						
Ethyl, 1-oxo- (Acetyl) + Nitrogen oxide (NO ₂)						
82 SLA/GUT	EX	295	(1.51±0.36)(13)			2
Flow-reactor. CH ₃ CO generated by reacting Cl atoms with CH ₃ CHO. Cl atoms generated by IR- multiphoton-induced decomposition of CF ₂ Cl ₂ . [CH ₃ CO] ₀ = (1.9-4.6)x10 ¹⁰ molec.cm ⁻³ . [CH ₃ CHO] = (5.7-6.5)x10 ¹⁴ molec.cm ⁻³ . [NO ₂] = (0-5)x10 ¹² molec.cm ⁻³ . P = (1-20) torr.						
CH ₃ CO + CH ₃ CO → CH ₃ C(O)C(O)CH ₃ (a)						
→ (CH ₃) ₂ CO + CO (b)						
→ CH ₃ CHO + CH ₂ =C=O (c)						
Ethyl, 1-oxo- (Acetyl)						
79 HAS/KOS	EX	298	2.37(13)			2
k _a . CH ₃ OOCH ₃ Flash-photolysis. Gas-chromatography. P = (1.5-700) torr.						

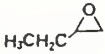
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 PAR k _a . Photolysis of Acetone at (25.4-40.0) nm. Molecular modulation spectroscopy.	EX	298	(1.81±0.60)(13)			2	
82 ANA/MAW k _a . Average of 24 k values obtained through a data-fit procedure. Molecular Modulation Spectroscopy. CH ₃ and CH ₃ CO produced by Azomethane/CO photolysis. P-independent k. [Azomethane] = 1.0x10 ¹⁷ molec.cm ⁻³ . [CO] = (0.3-2.7)x10 ¹⁹ molec.cm ⁻³ .	EX	263-343	(7.23±1.81)(12)	0	0	2	
82 TIM/KAL k _a . 2,3-Butanedione flash-photolysis. Gas-chromatography. [CH ₃ CO] = (1.14-5.77)x10 ¹⁸ molec.cm ⁻³ . P = (11-47) torr.	EX	298	(2.43±0.14)(13)			2	
78 ADA/BAS k _a + k _b + k _c . Acetone Flash-photolysis. Kinetic Spectroscopy. P(Total) = 50 torr.	ES	298	4.5(13)			2	
81 ADA/BAS2 k _a + k _b + k _c . Acetone Flash-photolysis. Kinetic Spectroscopy.	ES	298	3.5(13)			2	
CD ₃ CO + CD ₃ CO → CD ₃ C(O)C(O)CD ₃ (a) → (CD ₃) ₂ CO + CO (b) → CD ₃ CDO + CD ₂ =C=O (c)							
Ethyl-2,2,2-d ₃ , 1-oxo- (Acetyl)							
81 ADA/BAS2 k _a + k _b + k _c . Acetone-d ₆ Flash-photolysis. Kinetic Spectroscopy.	ES	298	3.4(13)			2	
CH ₃ CO + CH ₃ CHO → (CH ₃) ₂ CO + CHO							
Ethyl, 1-oxo- (Acetyl) + Acetaldehyde							
81 GIL/JOH Flash-photolysis of CH ₃ CHO. Time-resolved intracavity laser detection. P(CH ₃ CHO) = 0.2 torr.	EX	298	(1.71±0.37)(11)			2	
CH ₃ CO + CH ₂ =CHCH=CH ₂ → CH ₃ C(O)CH ₂ CHCH=CH ₂							
Ethyl, 1-oxo- + 1,3-Butadiene							
73 ENC/LIS k _{ref} : CH ₃ CO (+M) → CH ₃ + CO (+M)	RL	333-397	1.6(3)	0	-5284±503	2/1	5.01

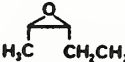
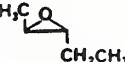
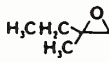
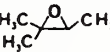
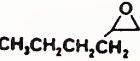
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{C}(\text{O})\text{O} + \text{NO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{O}_2\text{NO}_2$						
Ethoxy, 1-oxo- + Nitrogen oxide (NO_2)						
77 HEN/KEN	ES	298-318	6.3(11)	0	0	2
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO} \rightarrow \text{CH}_3 + \text{CO}_2 + \text{NO}_2$ (a)						
$\rightarrow \text{CH}_3\text{C}(\text{O})\text{O} + \text{NO}_2$ (b)						
Ethylldioxy, 1-oxo- + Nitrogen oxide (NO)						
76 COX/DER3	RL	296	(1.73±0.006)			2/2
k_a/k_{ref} .						
k_{ref} : $\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OONO}_2$						
77 HEN/KEN	RL	298-318	(3.1±0.5)	0	0	2/2
k_b/k_{ref} .						
k_{ref} : $\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OONO}_2$						
77 COX/ROF ¹⁾	ES	300	1.63(12)			2
77 HEN/KEN ¹⁾	RN	298-318	2.0(12)	0	0	2
¹⁾ k_b .						
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OONO}_2$ (a)						
$\rightarrow \text{any other products}$ (b)						
Ethylldioxy, 1-oxo- + Nitrogen oxide (NO_2)						
77 COX/ROF ¹⁾	RL	303-328	≈(5.4±1.7)(-1)			2/2
k_a/k_{ref} .						
Mean rate ratio.						
k_{ref} : $\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO} \rightarrow \text{CH}_3\text{C}(\text{O})\text{O} + \text{NO}_2$						
77 COX/ROF ¹⁾	DE	300	8.43(11)			2
k_a .						
Based on k/k_{ref} and Thermodynamic data.						
¹⁾ Thermolysis in a flow-reactor.						
80 ADD/BUR ²⁾	EX	302	(1.26±0.06)(12)			2
P = 28 torr.						
80 ADD/BUR ²⁾	EX	302	(2.83±0.18)(12)			2
P = 715 torr.						
²⁾ k_a .						
$\text{Cl}_2/\text{CH}_3\text{CHO}/\text{O}_2$ Modulated Photolysis.						
77 COX/DER3	RL	298	(2.4±1.4)(-1)			2/2
k_{overall}/k_a .						
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OOH} + \text{CHO}$						
Ethylldioxy, 1-oxo- + Formaldehyde						
74 DIX/SKI2	RL	392-461	(2.4±0.2)	0	0	2/2
Rate-ratio assumed to be T-independent.						
k_{ref} :						
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{CHO} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OOH} + \text{CH}_3\text{CO}$						

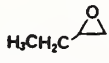
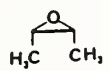
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃C(O)OO + CH₃C(O)OO						
→ CH ₃ O ₂ + CH ₃ O ₂ + CO ₂ + CO ₂ + O ₂ (a)						
→ any other products (b)						
Ethyldioxy, 1-oxo-						
80 ADD/BURR ¹⁾ k _a . Data-fit by computer simulation on the basis of a proposed mechanism.	DE	302	1.51(12)			2 2.0
80 ADD/BURR ¹⁾ k _{overall} . Weighted least-squares fit by assuming a simple second-order rate law.	EX	302	(3.9±1.8)(12)			2
¹⁾ Cl ₂ /CH ₃ CHO/O ₂ modulated photolysis.						
CH₃C(O)OO + CH₃CH=CH₂ → CH₃ + CO₂ + 						
Ethyldioxy, 1-oxo- + 1-Propene 77 DIA/SEL	RN	393	(6.40±0.36)(6)			2
CH₃C(O)OO + CH₃CH₂CH=CH₂ → CH₃ + CO₂ + 						
Ethyldioxy, 1-oxo- + 1-Butene						
74 DIA/WAD	RN	393	3.5(7)			2
75 SEL/WAD	RN	357-410	8.7(10)	0	3480±422	2 3.0
CH₃C(O)OO + cis-CH₃CH=CHCH₃						
→ CH ₃ + CO ₂ + 						
Ethyldioxy, 1-oxo- + 2-Butene, (Z)-						
72 RAY/WAD	ES	457	2.0(9)			2
75 DIA/SEL	RN	393	(7.5±0.1)(7)			2
CH₃C(O)OO + trans-CH₃CH=CHCH₃						
→ CH ₃ + CO ₂ + 						
Ethyldioxy, 1-oxo- + 2-Butene, (E)-						
75 DIA/SEL	RN	393	(1.2±0.1)(8)			2
CH₃C(O)OO + (CH₃)₂C=CH₂ → CH₃ + CO₂ + 						
Ethyldioxy, 1-oxo- + 1-Propene, 2-methyl-						
75 SEL/WAD	RN	357-410	1.9(11)	0	3012±141	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{cis-CH}_3\text{CH=CHCH}_2\text{CH}_3$ $\rightarrow \text{CH}_3 + \text{CO}_2 +$ 	RN	393	(1.41±0.84)(8)			2
Ethyldioxy, 1-oxo- + 2-Pentene, (Z)- 77 DIA/SEL						
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{trans-CH}_3\text{CH=CHCH}_2\text{CH}_3$ $\rightarrow \text{CH}_3 + \text{CO}_2 +$ 	RN	393	(1.41±0.84)(8)			2
Ethyldioxy, 1-oxo- + 2-Butene, (E)- 77 DIA/SEL						
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ $\rightarrow \text{CH}_3 + \text{CO}_2 +$ 	RN	393	5.0(8)			2
Ethyldioxy, 1-oxo- + 1-Butene, 2-methyl- 74 DIA/WAD						
77 DIA/SEL	RN	393	(1.52±0.08)(8)			2
$\text{CH}_3\text{C}(\text{O})\text{OO} + (\text{CH}_3)_2\text{CHCH=CH}_2$ $\rightarrow \text{CH}_3 + \text{CO}_2 +$ 	RN	393	(1.25±0.62)(7)			2
Ethyldioxy, 1-oxo- + 1-Butene, 3-methyl- 77 DIA/SEL						
$\text{CH}_3\text{C}(\text{O})\text{OO} + (\text{CH}_3)_2\text{C=CHCH}_3$ $\rightarrow \text{CH}_3 + \text{CO}_2 +$ 	RN	370-410	1.21(11)	0	1965±109	2 1.31
Ethyldioxy, 1-oxo- + 2-Butene, 2-methyl- 77 DIA/SEL						
77 DIA/SEL	RN	393	(8.38±0.84)(8)			2
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH=CH}_2$ $\rightarrow \text{CH}_3 + \text{CO}_2 +$ 	RN	393	(2.24±0.83)(7)			2
Ethyldioxy, 1-oxo- + 1-Hexene 77 DIA/SEL						

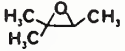
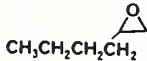
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃CHO (+ M) → CH₃ + CHO (+ M)							
Acetaldehyde							
73 BAR/MAR M = H ₂ . Based on analytical data.	EX	768-813	(3.88±2.94)(16)	0	40106±695	1	
73 BAR/MAR M = H ₂ . Based on pressure-time data.	EX	768-813	(8.87±4.42)(16)	0	41012±1636	1	
75 COL/NAE M = N ₂ .	EX	800-1225	7.08(15)	0	41155±503	1	1.62
76 ERN/SPI M = Ar. Limiting high-pressure k.	EX	1350-1650	1.2(16)	0	41137±481	1	
CH₃CHO + CH₃C(O)OOH → products							
Acetaldehyde + Ethaneperoxoic acid							
74 DIX/SKI1 ¹⁾	RN	336	2.0(-1)			2	
74 DIX/SKI1 ¹⁾	RN	345	1.9(-1)			2	
74 DIX/SKI1 ¹⁾	RN	393	4.45			2	
¹⁾ Surface/volume ratio = 0.6 cm ⁻¹ .							
74 DIX/SKI1 ²⁾	RN	345	7.3(-1)			2	
74 DIX/SKI1 ²⁾	RN	393	2.1(2)			2	
²⁾ Surface/volume ratio = 6.1 cm ⁻¹ .							
CH₃C(O)OOH + CH₃CH=CH₂ → CH₃COOH + 							
Ethaneperoxoic acid + 1-Propene							
77 DIA/SEL	RN	393	(2.32±0.86)			2	
CH₃C(O)OOH + CH₃CH₂CH=CH₂ → CH₃COOH + 							
Ethaneperoxoic acid + 1-Butene							
75 SEL/WAD	RN	357-410	4.8(11)	0	9915±1241	2	25.0
CH₃C(O)OOH + cis-CH₃CH=CHCH₃ → CH₃COOH + 							
Ethaneperoxoic acid + 2-Butene, (Z)-							
75 DIA/SEL Alkene added after CH ₃ CHO consumption.	RN	393	(3.0±0.7)(1)			2	
75 DIA/SEL Alkene added at the start of CH ₃ CHO + O ₂ reaction.	RN	393	(3.4±1.0)(1)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{trans-CH}_3\text{CH=CHCH}_3$						
$\rightarrow \text{CH}_3\text{COOH} + \begin{array}{c} \text{H}_3\text{C} \\ \diagup \quad \diagdown \\ \text{O} \\ \diagdown \quad \diagup \\ \text{CH}_3 \end{array}$						
Ethaneperoxoic acid + 2-Butene, (E)-						
75 DIA/SEL	RN	393	(3.0±0.7)(1)			2
Alkene added after CH_3CHO consumption.						
75 DIA/SEL	RN	393	(3.4±1.0)(1)			2
Alkene added at the start of $\text{CH}_3\text{CHO} + \text{O}_2$ reaction.						
$\text{CH}_3\text{C}(\text{O})\text{OOH} + (\text{CH}_3)_2\text{C=CH}_2$						
$\rightarrow \text{CH}_3\text{COOH} + \begin{array}{c} \text{O} \\ \diagup \quad \diagdown \\ \text{H}_3\text{C} \quad \text{C} \\ \diagdown \quad \diagup \\ \text{H}_3\text{C} \end{array}$						
Ethaneperoxoic acid + 1-Propene, 2-methyl-						
75 SEL/WAD	RN	357-410	4.3(10)	0	7939±1629	2
$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{cis-CH}_3\text{CH=CHCH}_2\text{CH}_3$						
$\rightarrow \text{CH}_3\text{COOH} + \begin{array}{c} \text{O} \\ \diagup \quad \diagdown \\ \text{H}_3\text{C} \quad \text{CH}_2\text{CH}_3 \end{array}$						
Ethaneperoxoic acid + 2-Pentene, (Z)-						
77 DIA/SEL	RN	393	(4.28±1.70)			2
$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{trans-CH}_3\text{CH=CHCH}_2\text{CH}_3$						
$\rightarrow \text{CH}_3\text{COOH} + \begin{array}{c} \text{H}_3\text{C} \\ \diagup \quad \diagdown \\ \text{O} \\ \diagdown \quad \diagup \\ \text{CH}_2\text{CH}_3 \end{array}$						
Ethaneperoxoic acid + 2-Pentene, (E)-						
77 DIA/SEL	RN	393	(4.38±1.70)			2
$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$						
$\rightarrow \text{CH}_3\text{COOH} + \begin{array}{c} \text{O} \\ \diagup \quad \diagdown \\ \text{H}_3\text{C} \quad \text{CH}_2\text{C}(\text{CH}_3) \\ \diagdown \quad \diagup \\ \text{H}_3\text{C} \end{array}$						
Ethaneperoxoic acid + 1-Butene, 2-methyl-						
77 DIA/SEL	RN	393	(6.03±2.16)(1)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{C}(\text{O})\text{OOH} + (\text{CH}_3)_2\text{CHCH}=\text{CH}_2$ $\rightarrow \text{CH}_3\text{COOH} +$ 							
Ethaneperoxoic acid + 1-Butene, 3-methyl-							
77 DIA/SEL	RN	393	(9.97±2.10)			2	
$\text{CH}_3\text{C}(\text{O})\text{OOH} + (\text{CH}_3)_2\text{C}=\text{CHCH}_3$ $\rightarrow \text{CH}_3\text{COOH} +$ 							
Ethaneperoxoic acid + 2-Butene, 2-methyl-							
77 DIA/SEL	RN	370-410	1.70(11)	0	7410±291	2	2.14
77 DIA/SEL	RN	393	(1.24±0.15)(3)			2	
$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ $\rightarrow \text{CH}_3\text{COOH} +$ 							
Ethaneperoxoic acid + 1-Hexene							
77 DIA/SEL	RN	393	(2.13±1.20)(1)			2	
$\text{CH}_3\text{CH}_2\text{O} \rightarrow \text{CH}_3 + \text{HCHO} \quad (\text{a})$ $\rightarrow \text{CH}_3\text{CHO} + \text{H} \quad (\text{b})$							
Ethoxy							
74 MOS/POL	RL	593	(1.4±0.2)(5)			1/2	
$k_{\text{ref}}:$ $\text{CH}_3\text{CH}_2\text{O} + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OH} + \text{CH}_2\text{CH}_3$							
77 BAT/MIL2 ¹⁾	ES	435-491	1.0(15)	0	10871	1	
79 BAT ¹⁾	ES	393-473	1.0(15)	0	10871±503	1	3.16
¹⁾ k_a .							
Conventional static system.							
77 BAT/MIL2 ²⁾	ES	435-491	2.51(14)	0	9763	1	
79 BAT ²⁾	ES	393-473	2.51(14)	0	11778	1	
²⁾ k_b .							
Conventional static system.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}_2\text{O} + \text{O}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2$						
Ethoxy + Oxygen molecule						
82 GUT/SAN ¹⁾	EX	296	4.8(9)			2
82 GUT/SAN ¹⁾	EX	353	5.9(9)			2
¹⁾ $\text{CH}_3\text{CH}_2\text{ONO}$ photolysis at 266 nm. Laser-induced Fluorescence. $P(\text{O}_2 + \text{N}_2) = 40$ torr.						
$\text{CH}_3\text{CH}_2\text{O} + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HNO}$ (a)						
$\rightarrow \text{CH}_3\text{CH}_2\text{ONO}$ (b)						
Ethoxy + Nitrogen oxide (NO)						
77 BAT/MIL2 k_a .	ES	435-491	6.31(12)	0	0±503	2 2.51
80 ROS k_a/k_{ref} . $\text{CH}_3\text{CH}_2\text{NO}_2/\text{NO}_2$ photolysis at 366 nm. k_{ref} : $\text{CH}_3\text{CH}_2\text{O} + \text{NO} \rightarrow \text{CH}_3\text{CH}_2\text{ONO}$	RL	298	(0.18±0.02)			2/2
77 BAT/MIL2 k_b . Same data in 74 BAT/MIL and 75 BAT/MCC.	ES	435-491	2.0(13)	0	0±503	2 2.51
$\text{CH}_3\text{CH}_2\text{O} + \text{NO}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HONO}$ (a)						
$\rightarrow \text{CH}_3\text{CH}_2\text{ONO}_2$ (b)						
Ethoxy + Nitrogen oxide (NO_2)						
77 BAT/MIL2 k_a .	ES	435-491	3.98(12)	0	0	2
80 ROS k_a/k_b . $\text{CH}_3\text{CH}_2\text{NO}_2/\text{NO}_2$ photolysis at 366 nm.	RL	298	(9.0±1.0)(-2)			2/2
77 BAT/MIL2 k_b .	ES	435-491	7.94(12)	0	0	2
$\text{CH}_3\text{CHOH} (+ \text{M}) \rightarrow \text{CH}_3\text{CHO} + \text{H} (+ \text{M})$						
Ethyl, 1-hydroxy-						
82 NAT/BHA M = O_2 + Ar. Ethanol/ O_2 /Ar ignition behind reflected shock-waves. Data-fit. P = (1-2) atm.	ES	1300-1700	5.00(13)	0	11000	2
$\text{CH}_3\text{CHOH} + \text{O}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2$ (a)						
$\rightarrow \text{CH}_3\text{CH}(\text{OH})\text{OO}$ (b)						
Ethyl, 1-hydroxy- + Oxygen molecule						
82 NAT/BHA k_a . M = O_2 + Ar. Ethanol/ O_2 /Ar ignition behind reflected shock-waves. Data-fit. P = (1-2) atm.	ES	1300-1700	1.00(13)	0	2800	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
81 WAS k _{overall} . Fast-flow reactor. Photoionization Mass-spectrometry. P(Ethanol) = 1.15 mtorr. P(Total) = 3.73 mtorr. P(O) ₀ = 9.78 mtorr. P(O) = 9.42 mtorr. k _{ref} : CD ₃ CDOH + ¹⁸ O → CD ₃ CDO + ¹⁸ OH (c) → CD ₃ CD ¹⁸ O → OH (d)	RL	298	(1.4±0.4)(-1)				2/2
CH ₃ CH ₂ O ₂ → HCHO + CH ₃ O (a) → CH ₃ CHO + OH (b) → CH ₂ CH ₂ OOH (c)							
Ethyldioxy							
74 MOS/POL k _a /k _b .	RL	593	1.34(1)				1/1
80 BAL/PIC k _c . Static system. Gas-chromatography.	ES	673-813	1.94(13)	0	17285±1208	1	3.16
CH ₃ CH ₂ O ₂ + NO → CH ₃ CH ₂ O + NO ₂							
Ethyldioxy + Nitrogen oxide (NO)							
79 ADA/BAS5 Azoethane/O ₂ /Ar photolysis. Kinetic-spectroscopy. [Azoethane] = (2.2-6.6)x10 ¹⁶ molec.cm ⁻³ . [O ₂] = (2.0-3.3)x10 ¹⁷ molec.cm ⁻³ . [Ar] = (1.1-2.5)x10 ¹⁸ molec.cm ⁻³ . [NO] = (0.2-2.1)x10 ¹⁵ molec.cm ⁻³ . Flash energy = 263cal.(1.1kJ).	EX	298	(1.6±0.1)(12)				2
82 PLU/RYA1 Flow-reactor. M = He. Mass-spectrometry. CH ₃ CH ₂ O ₂ generated by reacting Cl ₂ with CH ₃ CH ₃ and O ₂ in He, in a microwave discharge. [He] = 1.6x10 ¹⁷ molec.cm ⁻³ .	EX	295	(5.36±1.81)(12)				2
CH ₃ CH ₂ O ₂ + NO ₂ → products							
Ethyldioxy + Nitrogen oxide (NO ₂)							
79 ADA/BAS2 Flash-photolysis. Kinetic-spectroscopy. [Azoethane] < 3.0x10 ¹⁷ molec.cm ⁻³ . [Ar] ~ 1.2x10 ¹⁸ molec.cm ⁻³ . [O ₂] < 2.2x10 ¹⁹ molec.cm ⁻³ .	EX	298	(7.48±0.39)(11)				2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data	T/K	k, k/k(ref),	n	B,	k, A	k err.
$\text{CH}_3\text{CH}_2\text{O}_2 + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{O} + \triangle^{\text{O}}$							
Ethyldioxy + Ethene							
78 MOS/POL ¹⁾	ES	593	2.0(8)				2
78 MOS/POL ¹⁾	DE	653	1.1(9)				2
¹⁾ Static reactor. Gas-chromatography. Based on calculated $\text{CH}_3\text{CH}_2\text{O}_2$ concentrations.							
$\text{CH}_3\text{CH}_2\text{O}_2 + \text{CH}_3\text{CH}_2\text{O}_2 \rightarrow \text{CH}_3\text{CH}_2\text{O} + \text{CH}_3\text{CH}_2\text{O} + \text{O}_2$ (a) $\rightarrow \text{CH}_3\text{CHO} + \text{CH}_3\text{CH}_2\text{OH} + \text{O}_2$ (b) $\rightarrow \text{CH}_3\text{CH}_2\text{OOCH}_2\text{CH}_3 + \text{O}_2$ (c)							
Ethyldioxy							
79 ADA/BAS4	DE	298	(6.0±0.6)(10)				2
$k_a + k_b + k_c$. Flash-photolysis. Absorption-spectroscopy Computer data-fit.							
82 NIK/MAK2 ¹⁾	RL	298	1.3				2/2
k_a/k_b .							
82 NIK/MAK2 ¹⁾	RL	298	≤2.2(-1)				2/2
k_c/k_b .							
¹⁾ FTIR-Spectroscopy. $\text{CH}_3\text{CH}_2\text{O}_2$ generated by photolysis of an Azoethane/ O_2/N_2 mixture. [Azoethane] = 6.15×10^{14} molec.cm ⁻³ . P(N_2) = 650 torr. P(O_2) = 50 torr.							
$\text{CH}_3\text{CH}_2\text{OH} (+ \text{M}) \rightarrow \text{CH}_3 + \text{CH}_2\text{OH} (+ \text{M})$							
Ethanol							
76 TSA1	ES	1080-1165	2.51(6)	0	42500		1
82 NAT/BHA	CO	1300-1700	3.00(18)	0	38000		2
M = $\text{O}_2 + \text{Ar}$. Ethanol/ O_2/Ar ignition behind reflected shock-waves. Data-fit. P = (1-2) atm.							
$(\text{CH}_3)_2\text{O} \rightarrow \text{CH}_3\text{O} + \text{CH}_3$							
Methane, oxybis- (Dimethyl ether)							
75 PAC	EX	782-936	1.0(15)	0	38251±962	1	3.16
77 ARO/NAE1	EX	1063-1223	2.16(15)	0	38551	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 HEL/MAN Pyrolysis in a flow-reactor. UV-absorption-spectroscopy. Computer simulation. High-pressure k.	DE	1005	3.1(-2)			1	
78 ARO Pyrolysis in a flow reactor.	EX	1062-1223	2.16(15)	0	38551	1	
82 BAT/ALV (CH ₃) ₂ O pyrolysis with, or without CH ₄ . Static system. P(CH ₃ OCH ₃) = (400-800) torr.	EX	680-850	3.16(16)	0	41772±1007	1	6.31
CH₃OOCH₃ → CH₃O + CH₃O							
Peroxide, dimethyl-							
73 LIS/MAS	ES	400	3.3(-4)			1	
76 BAT/MCC1	EX	383-413	3.16(15)	0	18621±101	1	3.16
77 BAR/BEN1 Vacuum technique. Gas-chromatography.	EX	391-432	5.01(15)	0	18671±453	1	3.16
79 BAT/RAT ¹) k determined in presence of NO and CF ₄ .	EX	383-420	7.94(13)	0	16960±554	1	3.98
79 BAT/RAT ¹) k determined in presence of NO and NO ₂ .	EX	383-433	2.51(16)	0	19376±302	1	1.58
¹) Static system, with packed reaction vessels.							
$\Delta^S \rightarrow CH_2=CH_2 + S$							
Thiirane (Ethylene episulfide)							
82 AMA/YAM VLP-Pyrolysis. P < 10 ⁻⁵ torr.	EX	1030-1100	6.31(15)	0	21339	1	
$\Delta^S \rightarrow CH_2=CHSH$							
Thiirane (Ethylene episulfide)							
79 SHE/SAF ¹) k determined by experimental kinetics.	EX	298	5.0(10)			1	
79 SHE/SAF ¹) k calculated by RRKM theory.	CO	298	7.6(10)			1	
¹) COS UV-photolysis. High-vacuum system. Thiirane is in a vibrationally excited singlet ground state formed by S(¹ D ₂) + CH ₂ =CH ₂ .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{SCH}_2 + \text{CH}_4 \rightarrow (\text{CH}_3)_2\text{S} + \text{CH}_3$ Methyl, (methylthio)- + Methane							
76 ART/LEE Calculation based on the reverse reaction and Thermochemical data.	DE	393-518	6.31(1)	0	7662	2	
$\text{NCCN} (+ \text{M}) \rightarrow \text{CN} + \text{CN} (+ \text{M})$ Ethane dinitrile							
73 FUE/TAB M = Ar.	EX	2200-3700	(6.66±1.25)(16)	0	49643±609	2	
$\text{CH}_3\text{NC} \rightarrow \text{CH}_3\text{CN}$ Methane, isocyano-							
76 COL/PRI Thermal isomerization in static vessels. P = (2-100) torr.	EX	393-593	2.24(13)	0	19225±101	1	1.3
$(\text{CH}_3)_2\text{N} + \text{O}_2 \rightarrow \text{CH}_2=\text{NCH}_3 + \text{HO}_2$ Amidogen, dimethyl- + Oxygen molecule							
79 LIN/CAL ¹⁾ $k_{\text{ref}}: (\text{CH}_3)_2\text{N} + \text{NO} \rightarrow (\text{CH}_3)_2\text{NN}=\text{O}$	RL	298	(1.48±0.07)(-6)			2/2	
79 LIN/CAL ¹⁾ $k_{\text{ref}}: (\text{CH}_3)_2\text{N} + \text{NO}_2 \rightarrow (\text{CH}_3)_2\text{NNO}_2$ ¹⁾ Long-path, FTIR-spectroscopy.	RL	298	(3.90±0.28)(-7)			2/2	
$(\text{CH}_3)_2\text{N} + \text{NO}_2 \rightarrow \text{CH}_2=\text{NCH}_3 + \text{HONO}$ (a) $\rightarrow (\text{CH}_3)_2\text{NNO}_2$ (b) Amidogen, dimethyl- + Nitrogen oxide (NO ₂)							
79 LIN/CAL k_a/k_b . Long-path, FTIR-Spectroscopy.	RL	298	(2.2±0.6)(-1)			2/2	
$\text{CH}_3\text{N}=\text{NCH}_3 \rightarrow \text{CH}_3 + \text{CH}_3 + \text{N}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_3 + \text{N}_2$ (b) Diazene, dimethyl- (Azomethane)							
75 CAM/MAR k_a .	EX	676-813	2.00(13)	0	22734±481	1	2.0
78 MAR/PAG ¹⁾ k_a .	EX	534-657	7.94(13)	0	23287±301	1	1.66

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units factor	k err. factor
78 MAR/PAG ¹⁾ k _b . ¹⁾ Azomethane pyrolysis in a static vacuum system. P = (50-150) torr.	EX	534-657	3.39(11)	0	22193±854	1	3.89
$\text{CH}_3\text{N}=\text{NCH}_3^* \rightarrow \text{CH}_3 + \text{CH}_3 + \text{N}_2$ Diazene, dimethyl- (Azomethane)							
77 CHE/ORE Azomethane/He high-P photolysis. RRKM data-fit to a proposed mechanism. Azomethane assumed to be in a vibrationally excited T ₁ electronic state. Lower-limit k. (He) = (0-100) atm.	CO	298	>4.0(10)			1	
$(\text{CH}_3)_2\text{NNH}_2 \rightarrow (\text{CH}_3)_2\text{N} + \text{NH}_2$ Hydrazine, 1,1-dimethyl-							
72 GOL/SOL RRKM fit of experimental data.	EX	869-1076	3.98(17)	0	31706	1	
$\text{CH}_3\text{NHNHCH}_3 \rightarrow \text{CH}_3\text{N}=\text{NCH}_3 + \text{H}_2$ Hydrazine, 1,2-dimethyl-							
72 GOL/SOL RRKM fit of experimental data.	EX	910-1271	3.16(13)	0	28686	1	
$\text{CH}_3\text{COOONO}_2 \rightarrow \text{CH}_3\text{COOO} + \text{NO}_2$ Peroxide, acetyl nitro-							
77 COX/ROF Thermolysis in a flow reactor.	EX	294-328	7.94(14)	0	12510±385	1	3.98
77 HEN/KEN	EX	298-313	1.95(16)	0	13543±453	1	3.98
77 HEN/KEN	EX	298	(4.0±0.9)(-4)			1	
$\text{CH}_3\text{CH}_2\text{NO} + \text{CH}_3\text{CH}_2\text{NO} \rightarrow (\text{CH}_3\text{CH}_2\text{NO})_2$ Ethane, nitroso-							
72 TAN/LAM	EX	314	(3.01±0.30)(4)			2	
$\text{CH}_3\text{CH}_2\text{NO}_2 (+\text{M}) \rightarrow \text{CH}_3\text{CH}_2 + \text{NO}_2 (+\text{M})$ Ethane, nitro-							
73 GLA/TRO ¹⁾ Limiting high-pressure k.	EX	900-1350	7.94(15)	0	28686	1	
73 GLA/TRO ¹⁾ Limiting low-pressure k.	EX	900-1350	1.0(18)	0	18118	2	
¹⁾ Thermolysis in shock waves. Conc.(Ar): (0.027-1.807)10 ²⁰ molec.cm ⁻³ .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{CH}_2\text{ONO} \rightarrow \text{CH}_3\text{CHO} + \text{HNO}$ (a)							
$\rightarrow \text{CH}_3\text{CH}_2\text{O} + \text{NO}$ (b)							
Nitrous acid ethyl ester (Ethyl nitrite)							
75 BAT/MCC ¹⁾	ES	393-473	6.31(13)	0	18873	1	
77 BAT/MIL2 ¹⁾	ES	435-491	5.01(13)	0	18873	1	
78 BAT/ISL2 ¹⁾	EX	433-473	7.94(14)	0	20081±503	1	3.16
Pyrolysis in a static system.							
Gas-chromatography.							
¹⁾ k_a .							
77 BAT/MIL2	ES	435-491	1.0(16)	0	21037±453	1	2.51
k_b .							
Same data given in 74 BAT/MIL and 75 BAT/MCC.							
$\text{CH}_3\text{CH}_2\text{ONO}_2 \rightarrow \text{CH}_3\text{CH}_2 + \text{NO}_2$							
Nitric acid ethyl ester (Ethyl nitrate)							
77 BAT/MIL2	ES	435-491	1.0(16)	0	20131	1	
$\text{C}_3 + \text{O}_2 \rightarrow \text{C}_2(\text{d}^3\Pi, v=1) + \text{CO} + \text{O}$ (or CO_2) (a)							
$\rightarrow$ any other product (b)							
Carbon trimer + Oxygen molecule							
77 MAN	EX	2470	≥1.20(12)			2	
k_a . High-T flowing system.							
Lower-limit k.							
80 LES/HIC	EX	298	≤9.03(9)			2	
k_{overall} . Laser-induced fluorescence.							
Upper-limit k.							
80 REI/MAN1	EX	300	≤1.20(10)			2	
k_{overall} . Upper-limit k.							
IR Multiphoton dissociation of Allene.							
82 NEL/HEL	EX	295-610	≤1.20(8)			2	
k_{overall} . C_3 generated by multiphoton							
UV-photolysis of C_6H_6 at 249 nm.							
Laser-induced Fluorescence.							
Upper-limit k.							
P(Total) = (5-100) torr.							
P(C_6H_6) = (1-2) mtorr.							
P(O) = 90 torr.							
$\text{C}_3 + \text{N}_2 \rightarrow$ products							
Carbon trimer + Nitrogen molecule							
80 REI/MAN1	EX	300	≤1.81(10)			2	
IR-Multiphoton dissociation of Allene.							
Upper-limit k.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
C₃ + NO → products						
Carbon trimer + Nitrogen oxide (NO)						
80 LES/HIC Dye-laser induced fluorescence.	EX	298	1.26(11)			2
80 REI/MAN1 IR Multiphoton dissociation of 1,2-Propadiene. Upper-limit k.	EX	300	≤1.81(10)			2
C₃ + CH₄ → products						
Carbon trimer + Methane						
80 REI/MAN1 IR-Multiphoton dissociation of Allene. Upper-limit k.	EX	300	≤1.81(10)			2
82 NEL/HEL C ₃ generated by Multiphoton Laser-photolysis of C ₆ H ₆ at 249 nm. Laser-induced fluorescence. Upper-limit k. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr. P(CH ₄) = 90 torr.	EX	295-610	≤3.01(8)			2
C₃ + CH≡CH → products						
Carbon trimer + Ethyne						
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser photolysis of C ₆ H ₆ . Laser-induced Fluorescence. Upper-limit k. P(CH≡CH) = (0-50) torr.	EX	294	<6.02(8)			2
82 NEL/HEL C ₃ generated by multiphoton UV-photolysis of C ₆ H ₆ at 249 nm. Laser-induced Fluorescence. Probable Products: C ₃ H + CH≡C. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr. P(CH≡CH) = (0-30) torr.	EX	295-610	(5.47±1.61)(12)	0	4065±161	2
C₃ + CH₂=CH₂ → products						
Carbon trimer + Ethene						
81 NEL/PAS C ₃ is generated by multiphoton UV excimer laser photolysis of C ₆ H ₆ . Laser-induced Fluorescence. Upper-limit k. P(CH ₂ =CH ₂) = (0-68) torr.	EX	294	<6.02(8)			2
82 NEL/HEL C ₃ generated by multiphoton UV-photolysis of C ₆ H ₆ at 249 nm. Laser-induced Fluorescence. Probable products: C ₃ H + CH ₂ =CH. P(Total) = (5-100) torr. P(CH ₂ =CH ₂) = (0-50) torr. P(C ₆ H ₆) = (1-2) torr.	EX	295-610	(1.03±0.31)(12)	0	3277±168	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
C₃ + CH₃CH₃ → products						
Carbon trimer + Ethane						
80 REI/MAN1 IR-Multiphoton dissociation of Allene. Upper-limit k.	EX	300	≤1.81(10)			2
C₃ + CH₃C≡CH → products						
Carbon trimer + 1-Propyne						
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-Fluorescence. P(CH ₃ C≡CH) = (0-2.8) torr.	EX	294	(1.98±0.04)(11)			2
82 NEL/HEL C ₃ generated by multiphoton UV-Photolysis of C ₆ H ₆ at 249 nm. Laser-induced fluorescence. P(Total) = (5-100) torr. P(CH ₃ C≡CH) = (0-1) torr. P(C ₆ H ₆) = (1-2) mtorr.	EX	295-610	(2.97±0.28)(12)	0	121±35	2
C₃ + CH₂=C=CH₂ → products						
Carbon trimer + 1,2-Propadiene (Allene)						
80 LES/HIC Dye-laser induced fluorescence.	EX	298	2.59(11)			2
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-induced Fluorescence. P(Allene) = (0-3.71) torr.	EX	294	(5.36±0.36)(10)			2
C₃ + CH₃CH=CH₂ → products						
Carbon trimer + 1-Propene						
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-induced Fluorescence. P(CH ₃ CH=CH ₂) = (0-6.0) torr.	EX	294	(3.03±0.19)(10)			2
82 NEL/HEL C ₃ generated by multiphoton UV-Photolysis of C ₆ H ₆ at 249 nm. Laser-induced Fluorescence. P(CH ₃ CH=CH ₂) = (0-6.25) torr. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr.	EX	295-610	(6.26±0.36)(10)	0	159±21	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$C_3 + CH_3CH_2CH=CH_2 \rightarrow$ products						
Carbon trimer + 1-Butene						
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-induced Fluorescence. P(CH ₃ CH ₂ CH=CH ₂) = (0-4.8) torr.	EX	294	(5.52±0.37)(10)			2
82 NEL/HEL C ₃ generated by multiphoton UV-Photolysis of C ₆ H ₆ at 249 nm. Laser-induced fluorescence. P(1-Butene) = (0-7) torr. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr.	EX	295-610	(7.34±0.30)(10)	0	139±17	2
$C_3 + \text{cis-}CH_3CH=CHCH_3 \rightarrow$ products						
Carbon trimer + 2-Butene, (Z)-						
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-induced Fluorescence. P(cis-2-Butene) = (0-0.98) torr.	EX	294	(2.51±0.08)(11)			2
82 NEL/HEL C ₃ generated by multiphoton UV-Photolysis of C ₆ H ₆ at 249 nm. Laser-induced Fluorescence. P(cis-2-Butene) = (0-1) torr. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr.	EX	295-610	(1.26±0.06)(11)	0	-201±19	2
$C_3 + (CH_3)_2C=CH_2 \rightarrow$ products						
Carbon trimer + 1-Propene, 2-methyl-						
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-induced Fluorescence. P(Isobutene) < 0.082 torr.	EX	294	(2.91±0.11)(12)			2
82 NEL/HEL C ₃ generated by multiphoton UV-photolysis of C ₆ H ₆ at 249 nm. Laser-induced Fluorescence. P(2-Methyl-1-propene) = (0-0.08) torr. P(Benzene) = (1-2) mtorr. P(Total) = (5-100) torr.	EX	295-610	(2.53±0.10)(11)	0	-759±15	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$C_3 + CH_3CH_2CH_2CH_3 \rightarrow$ products						
Carbon trimer + Butane						
82 NEL/HEL C_3 generated by Multiphoton UV-photolysis of C_6H_6 at 249 nm. Laser-induced fluorescence. Upper-limit k. $P(Total) = (5-100)$ torr. $P(C_6H_6) = (1-2)$ mtorr. $P(Butane) = 90$ torr.	EX	295-610	$\leq 1.20(8)$			2
$C_3 + CH_3CH_2CH_2C\equiv CH \rightarrow$ products						
Carbon trimer + 1-Pentyne						
81 NEL/PAS C_3 generated by multiphoton UV excimer laser Photolysis of C_6H_6 . Laser induced Fluorescence. $P(1-Pentyne) = (0-0.48)$ torr.	EX	294	$(3.37 \pm 0.19)(11)$			2
$C_3 + CH_3CH=C=CHCH_3 \rightarrow$ products						
Carbon trimer + 2,3-Pentadiene						
81 NEL/PAS C_3 generated by multiphoton UV excimer laser Photolysis of C_6H_6 . Laser-induced Fluorescence. 2,3-Pentadiene form unspecified (cis, or trans). $P(2,3-Pentadiene) = (0-0.4)$ torr.	EX	294	$(6.45 \pm 0.54)(11)$			2
$C_3 + (CH_3)_2C=CHCH_3 \rightarrow$ products						
Carbon trimer + 2-Butene, 2-methyl-						
81 NEL/PAS C_3 generated by multiphoton UV excimer laser Photolysis of C_6H_6 . Laser-induced Fluorescence. $P(2-Methylbut-2-ene) = (0-0.044)$ torr.	EX	294	$(8.97 \pm 0.60)(12)$			2
82 NEL/HEL C_3 generated by multiphoton UV-photolysis of C_6H_6 at 249 nm. Laser-induced Fluorescence. $P(2-Methyl-2-Butene) = 90$ torr. $P(Total) = (5-100)$ torr. $P(C_6H_6) = (1-2)$ mtorr.	EX	295-610	$(3.35 \pm 0.27)(11)$	0	-1014 ± 34	2
$C_3 + CH_3CH_2CH_2C\equiv CCH_3 \rightarrow$ products						
Carbon trimer + 2-Hexyne						
81 NEL/PAS C_3 generated by multiphoton UV excimer laser Photolysis of C_6H_6 . Laser-induced Fluorescence. $P(2-Hexyne) = (0-0.1)$ torr.	EX	294	$(4.01 \pm 0.18)(12)$			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k(k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
82 NEL/HEL C ₃ generated by multiphoton UV-photolysis of C ₆ H ₆ at 249 nm. Laser-induced fluorescence. P(2-Hexyne) = (0-0.07) torr. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr.	EX	295-610	(6.50±0.05)(11)	0	-695±25	2	
C ₃ + (CH ₃) ₂ C=C(CH ₃) ₂ → products Carbon trimer + 2-Butene, 2,3-dimethyl-							
82 NEL/HEL C ₃ generated by multiphoton UV-photolysis of C ₆ H ₆ at 249 nm. Laser-induced fluorescence. P(2,3-Dimethyl-2-butene) = (0-0.08) torr. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr.	EX	295-610	(1.26±0.11)(12)	0	-917±33	2	
C ₃ + (CH ₃) ₂ C=C(CH ₃) ₂ → products Carbon trimer + 2,3-Pentadiene, 2,4-dimethyl-							
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-induced Fluorescence. P(2,4-Dimethylpenta-2,3-diene) = (0-0.07) torr.	EX	294	(3.15±0.94)(12)			2	
CH ₃ C≡CD → CH ₂ =C=CHD (a) → CH ₂ DC=CH (b)							
1-Propyne-d							
80 HOP/PRI 1) k _a /k _b . Best data-fit.	RL	853-1033	2.86(-1)			1/1	
80 HOP/PRI 1) k _a + k _b .	EX	853-1033	1.26(11)	0	28334±604	1	2.0
1) CH ₃ C≡CD pyrolysis in a flow-reactor. P(N ₂) = 760 torr.							
CH ₂ DC=CH → CH ₃ C≡CD (a) → CH ₂ =C=CHD (b)							
1-Propyne-3-d							
80 HOP/PRI 1) k _a /k _{ref} .	RL	853-1033	3.33(-1)			1/1	
80 HOP/PRI 1) k _b /k _{ref} .	RL	853-1033	2.50(-1)			1/1	
1) CH ₃ C≡CD pyrolysis in a flow-reactor. P(N ₂) = 760 torr. Best data-fit. k _{ref} : CH ₃ C≡CD → CH ₂ DC=CH.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2=\text{C}=\text{CH}_2 (+\text{M}) \rightarrow \text{CH}_3\text{C}=\text{CH} (+\text{M})$ (a)						
$\rightarrow \triangle (+\text{M})$ (b)						
1,2-Propadiene (Allene)						
75 BRA/WES k_a . M = Ar. Limiting high-pressure k.	EX	1440-1700	3.02(14)	0	46670±1925	1 3.63
75 LIF/FRE2 k_a . M = Ar.	EX	1030-1220	1.48(13)	0	30398±1560	1 3.98
78 SIM/MEL k_a . Allene isomerization. Single-pulse shock-tube. M = Ar. P(Total) = 2 atm.	EX	1156-1172	(1.78±0.11)(1)	0	0	1
78 BAI/WAL k_b . Allene cyclization. Pyrolysis in a static system. P(Total) ~ 413 torr.	EX	466-516	1.12(13)	0	32056	1
$\text{CH}_2=\text{C}=\text{CHD} \rightarrow \text{CH}_3\text{C}=\text{CD}$ (a)						
$\rightarrow \text{CH}_2\text{DC}=\text{CH}$ (b)						
1,2-Propadiene-1-d						
80 HOP/PRI ¹⁾ k_a/k_{ref} .	RL	853-1033	2.46(-1)	0	0	1/1
80 HOP/PRI ¹⁾ k_b/k_{ref} .	RL	853-1033	6.47(-1)	0	0	1/1
¹⁾ Pyrolysis in a flow-reactor. Best data-fit. k_{ref} : $\text{CH}_3\text{C}=\text{CD} \rightarrow \text{CH}_2\text{DC}=\text{CH}$. P(N ₂) = 760 torr.						
$\triangle \rightarrow \text{CH}_3\text{C}=\text{CH}$ (a)						
$\rightarrow \text{CH}_2=\text{C}=\text{CH}_2$ (b)						
Cyclopropene						
78 BAI/WAL ²⁾ k_a .	EX	466-516	1.23(13)	0	18776±49	1 1.09
78 BAI/WAL ²⁾ k_a . Limiting high-pressure k. Adjusted value on the basis of theory.	EX	466-516	1.78(13)	0	18861	1
78 BAI/WAL ²⁾ k_b .	EX	466-516	1.78(13)	0	21810	1
²⁾ Pyrolysis in a static system. P(Total) 413 torr.						
$\text{CH}_3\text{CH}=\text{CH}^\dagger \rightarrow \text{CH}_2\text{CH}=\text{CH}_2^\dagger$						
1-Propenyl						
74 IBU/MUR ¹⁾	EX	402	4.04(7)			1
74 IBU/MUR ¹⁾	EX	453	8.38(7)			1
¹⁾ $\text{CH}_3\text{CH}=\text{CH}^\dagger$ formed by $\text{CH}_3 + \text{CH}=\text{CH}$.						

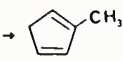
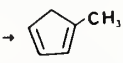
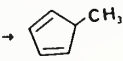
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2=\text{CHCH}_2^\dagger \rightarrow \text{CH}_2=\text{C}=\text{CH}_2 + \text{H}$						
2-Propenyl (Allyl)						
78 WIE/COL ¹⁾ At 7.1 eV.	EX	298	(5.1±0.3)(6)			1
78 WIE/COL ¹⁾ At 7.6 eV.	EX	298	(1.28±0.07)(7)			1
¹⁾ Photolysis. Static system. Gas-chromatography. $\text{CH}_2=\text{CHCH}_2^\dagger$ formed in photolysis of 1-Pentene by $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2^{**} \rightarrow \text{CH}_2=\text{CHCH}_2^\dagger + \text{CH}_3\text{CH}_2$						
$\text{CD}_2=\text{CDCH}_2^\dagger \rightarrow \text{CD}_2=\text{C}=\text{CD}_2 + \text{D}$						
2-Propenyl-1,1,2,3,3-d ₅ (Allyl-d ₅)						
78 WIE/COL ¹⁾ At 7.1 eV.	EX	298	(3.4±0.3)(6)			1
78 WIE/COL ¹⁾ At 7.6 eV.	EX	298	(7.5±0.5)(6)			1
¹⁾ Photolysis. Static system. Gas-chromatography. $\text{CD}_2=\text{CDCH}_2^\dagger$ formed in photolysis of 1-Pentene-d ₁₀ by $\text{CD}_3\text{CD}_2\text{CD}_2\text{CD}=\text{CD}_2^{**} \rightarrow \text{CD}_2=\text{CDCH}_2^\dagger + \text{CD}_3\text{CD}_2$						
$\text{CH}_2=\text{CHCH}_2 + \text{O}_2 \rightarrow \text{CH}_2=\text{CHCH}_2\text{O}_2$						
2-Propenyl (Allyl) + Oxygen molecule						
81 RUI/BAY M = He. Photoionization Mass-spectrometry. Flash-Photolysis of 1,5-Hexadiene/O ₂ at 193 nm. with an ArF excimer laser. P(Total) = 2.8 torr. P(1,5-Hexadiene) ~100 mtorr. P(O ₂) = (4.1-27.4) mtorr.	EX	348	(9.51±1.91)(10)			2
$\text{CH}_2=\text{CHCH}_2 + \text{NO} (+ \text{M}) \rightarrow \text{C}_3\text{H}_5\text{NO} (+ \text{M})$						
2-Propenyl (Allyl) + Nitrogen oxide (NO)						
82 TUL/MAC ¹⁾ ³⁾	EX	295	(8.13±0.18)(12)			2
82 TUL/MAC ¹⁾ ³⁾	EX	350	(6.74±0.24)(12)			2
82 TUL/MAC ¹⁾ ³⁾	EX	404	(5.60±0.18)(12)			2
¹⁾ Limiting high-pressure k.						
82 TUL/MAC ²⁾ ³⁾	EX	295	(1.45±0.62)(19)			3
82 TUL/MAC ²⁾ ³⁾	EX	350	(9.07±3.63)(18)			3
82 TUL/MAC ²⁾ ³⁾	EX	404	(5.80±2.18)			3
(The product is probably $\text{CH}_2=\text{CHCH}_2\text{NO}$)						
²⁾ Limiting low-pressure k.						
³⁾ M = Ar. 1,5-Hexadiene/NO/Ar flash-photolysis. P(Total) = (50-500) torr. P(NO) = (20-100) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2=\text{CHCH}_2 + \text{NO}_2 \rightarrow \text{CH}_2=\text{CHCH}_2\text{O} + \text{NO}$ (a)						
$\rightarrow \text{CH}_2=\text{C}=\text{CH}_2 + \text{HONO}$ (b)						
2-Propenyl (Allyl) + Nitrogen oxide (NO_2)						
81 SLA/YAM	EX	300	(2.34±0.48)(13)			2
$k_a + k_b$. Allyl radicals generated by pulsed IR-Multiphoton-induced decomposition of Allyl bromide in a tubular reactor. Photoionization Mass-spectrometry. Detection problems prevented determination of channel (b) products.						
$[\text{NO}_2]_0 = 3.3 \times 10^{12} \text{ molec.cm}^{-3}$. $P = 1 \text{ torr}$.						
$[\text{CH}_2=\text{CHCH}_2]_0 < 1.0 \times 10^{11} \text{ molec.cm}^{-3}$.						
$\text{CH}_2=\text{CHCH}_2 + \text{CH}=\text{CH} \rightarrow \left[\text{Cyclopentadienyl}^\bullet \right] \rightarrow \text{Cyclopentadiene} + \text{H}$						
2-Propenyl (Allyl) + Ethyne $\rightarrow$ [3-Cyclopenten-1-yl]						
$\rightarrow$ 1,3-Cyclopentadiene + Hydrogen atom						
81 NOH/SAK ¹⁾	ES	723-783	3.98(14)	0	12509	2
81 NOH/SAK ¹⁾	ES	773	4.37(7)			2
¹⁾ Pyrolysis of Ethanedioic acid di-2-propenyl ester, followed by cycloaddition in a flow-reactor. Mass-spectrometry.						
Same data given in 80 NOH/SAK.						
$\text{CH}_2=\text{CHCH}_2 + \text{CH}_2=\text{CH}_2 \rightarrow \left[\text{Cyclopentadienyl}^\bullet \right] \rightarrow \text{Cyclopentadiene} + \text{H}$ (a)						
$\rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_3$ (b)						
2-Propenyl (Allyl) + Ethene $\rightarrow$ [Cyclopentyl]						
$\rightarrow$ Cyclopentene + Hydrogen atom (a)						
$\rightarrow$ 1-Pentene (b)						
81 NOH/SAK ¹⁾	ES	723-783	5.89(9)	0	5774	2
k_a .						
81 NOH/SAK ¹⁾	ES	773	3.31(6)			2
k_a .						
81 NOH/SAK ¹⁾	ES	723-783	1.26(11)	0	8396	2
k_b .						
81 NOH/SAK ¹⁾	ES	773	2.40(6)			2
k_b . For channel (b), the intermediate (Cyclopentyl) abstracts a H atom from any RH to form 1-Pentene.						
¹⁾ Pyrolysis of Ethanedioic acid di-2-propenyl ester followed by cycloaddition in a flow-reactor. Mass-spectrometry.						
Same data in given 80 NOH/SAK.						

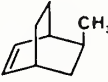
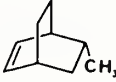
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2=\text{CHCH}_2 + \text{CH}\equiv\text{CCH}_3 \rightarrow \left[\text{Cyclopentadienyl}^\bullet\text{-CH}_3 \right]$						
→  + H (a)						
→  + H (b)						
→  + H (c)						
→  + CH ₄ (d)						
→ CH ₂ =CHCH ₂ CH=CHCH ₃ (e)						
→ CH ₂ =CHCH ₂ C(CH ₃)=CH ₂ (f)						
2-Propenyl (Allyl) + 1-Propyne						
→ [3-Cyclopenten-1-yl, 3-methyl-]						
→ 1,3-Cyclopentadiene, 2-methyl- + H atom (a)						
→ 1,3-Cyclopentadiene, 1-methyl- + H atom (b)						
→ 1,3-Cyclopentadiene, 5-methyl- + H atom (c)						
→ 1,3-Cyclopentadiene + Methane (d)						
→ 1,4-Hexadiene (e)						
→ 1,4-Pentadiene, 2-methyl- (f)						
81 NOH/SAK ¹) ⁶)	ES	723-783	7.94(13)	0	12269	2
81 NOH/SAK ¹) ⁶)	ES	773	9.33(6)			2
¹) k _a .						
81 NOH/SAK ²) ⁶)	ES	723-783	1.26(14)	0	12870	2
81 NOH/SAK ²) ⁶)	ES	773	7.76(6)			2
²) k _b .						
81 NOH/SAK ³) ⁶)	ES	723-783	2.00(14)	0	14073	2
81 NOH/SAK ³) ⁶)	ES	773	2.24(6)			2
³) k _c .						
81 NOH/SAK ⁴) ⁶)	ES	723-783	2.5(13)	0	12028	2
81 NOH/SAK ⁴) ⁶)	ES	773	4.07(6)			2
The intermediate abstracts a H atom from any RH to form 1,3-Cyclopentadiene and Methane.						
⁴) k _d .						
81 NOH/SAK ⁵) ⁶)	ES	723-783	7.94(11)	0	9659	2
81 NOH/SAK ⁵) ⁶)	ES	773	3.24(6)			2
The intermediate abstracts a H atom from any RH to form 1,4-Hexadiene.						
⁵) k _e .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 NOH/SAK ⁶⁾ k _f . The intermediate abstracts a H atom from any RH to form 2-Methyl-1,4-pentadiene. ⁶⁾ Pyrolysis of Ethanedioic acid di-2-propenyl ester, followed by cycloaddition in a flow-reactor. Gas-chromatography. Mass-spectrometry. The intermediate is 3-Methylcyclopent-3-en-1-yl radical.	ES	773	1.48(6)			2	
$\text{CH}_2=\text{CHCH}_2 + \text{CH}_2=\text{CHCH}_2 \rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CH}_2$							
2-Propenyl (Allyl)							
79 ROS/KIN ¹⁾	EX	625	(6.5±1.0)(12)			2	
79 ROS/KIN ¹⁾ Average of 7 k's determined at various temperatures within the 844-922 K range.	EX	880	(1.9±0.8)(12)			2	
¹⁾ VLP-pyrolysis.							
82 TUL/MAC 2-Propenyl generated by 1,5-Hexadiene Flash-photolysis in Ar. P(1,5-Hexadiene) = (0.04-1.0) torr. P(Ar) = (0-250) torr.	EX	293-571	(1.02±0.02)(13)	0	-132±12	2	
$\text{CH}_3\text{CH}=\text{CH}_2 (+\text{M}) \rightarrow \text{CH}_3 + \text{CH}_2=\text{CH} (+\text{M})$ (a) → any other products (b)							
1-Propene							
74 BAK/NOV k _{overall} .	EX	973-1123	2.3(14)	0	37141±1510	1	
75 BUR k _a . M = Ar. Concentration-dependent k, with Arrhenius expression = k/[Ar].	EX	1160-1700	1.0(13)	0	37242±503	2	3.16
82 KIE/ALA ¹⁾ The preexponential factor expressed as: A(T/298) ^{-15.7} .	EX	1650-2300	7.71(36)	-15.7	60393	2	
82 KIE/ALA ¹⁾ ¹⁾ k _a . M = Kr, or 1-Propene. Pyrolysis of 1-Propene behind incident shock-waves. Laser-schlieren. k derived from a simulation-assisted extrapolation-measured density gradient to the presumed instant of shock-heating. [M] = (0.6-1.3)×10 ¹⁸ molec.cm ⁻³ . P = (2.8-10.3) torr.	DE	2000	6.20(10)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}=\text{CH}_2 \uparrow \rightarrow \text{H} + \text{CH}_2=\text{CHCH}_2$						
1-Propene						
80 IBU/TAK Decomposition of chemically activated 1-Propene, generated by combination of CH_3 with $\text{CH}_2=\text{CH}$. CH_3 generated by the Hg-photosensitized decomposition of CH_4 . $\text{CH}_2=\text{CH}$ generated by combination of H with $\text{CH}\equiv\text{CH}$.	EX	288	(5.04±0.11)(7)			1
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2\text{CH}=\text{CH}_2 + (\text{CH}_3)_2\text{CH} \text{ (a)}$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 \text{ (b)}$ $\rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}=\text{CH}_2 \text{ (c)}$						
1-Propene						
73 SIM/BAC k_a .	EX	743-803	2.51(13)	0	21892	2
78 RIC/BAC $k_b = k_c$. Pyrolysis in a static system. P(olefin) = (33-300) torr.	EX	682-754	3.55(9)	0	18621±503	2 2.0
$\text{CH}_3\text{CH}=\text{CH}_2 + $  $\rightarrow $  $\text{CH}_3 \text{ (a)}$ $\rightarrow $  $\text{CH}_3 \text{ (b)}$						
1-Propene + 1,3-Cyclohexadiene $\rightarrow$ $\rightarrow$ Bicyclo[2.2.2]oct-2-ene, 5-methyl- (1 α ,4 α ,5 α)- (Exo form) (a) $\rightarrow$ Bicyclo[2.2.2]oct-2-ene, 5-methyl-, (1 α ,4 α ,5 β)- (Endo form) (b)						
74 DEB/HUY ¹⁾ k_a .	EX	512-638	4.57(9)	0	15143±40	2 1.07
74 DEB/HUY ¹⁾ k_b .	EX	512-638	5.50(8)	0	13120±40	2 1.07
¹⁾ Addition of Propene to 1,3-Cyclohexadiene in a cylindrical Pyrex reaction vessel. Gas-chromatography. Mass-spectrometry. P = (70-640) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\triangle \rightarrow \text{CH}_2\text{CH}=\text{CH}_3$ (a)						
$\rightarrow$ any other products (b)						
Cyclopropane						
73 DOR/CRO k_a . M = Ar. Cyclopropane thermal isomerization behind reflected shock-waves.	EX 1158-1323		5.0(9)	0	16104	1 3.0
78 TSA2 ¹⁾ k_a . P = 1.7 Atm.	EX 1000-1200		1.26(14)	0	31100±200	1 1.26
78 TSA2 ¹⁾ k_a . P = 5.0 Atm.	EX 1000-1200		2.0(14)	0	31100±100	1 1.26
¹⁾ Cyclopropane Thermolysis in a single-pulse shock-tube in Ar, in presence of Cyclohexane and Toluene. k's determined relative to the reaction:						
 $\rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CH}_2=\text{CH}_2$						
[Cyclopropane] = 0.01%. [Cyclohexene] = 0.01%. P(Ar) ~ (1.7-7) atm. [Toluene] = 1%.						
71 DOR/MCG k_a . M = He + Ar. Cyclopropane isomerization to 1-Propene behind reflected shock-waves. Limiting high-pressure k. [Cyclopropane] = (0.1-1.0)% P ₀ = (103-259) torr.	EX 935-1397		3.16(14)	0	32763±403	1 1.38
73 JEF/DAS k_a . M = Ar. Cyclopropane thermal isomerization in a single-pulse shock-tube. Measurement rela- tive to the Cyclohexane decomposition. Gas-chromatography.	RN 980-1040		1.82(15)	0	33669	1
73 JEF/LEW k_a . M = Ar. Cyclopropane Thermal isomerization behind reflected shock-waves, in a single-pulse shock-tube. Limiting high-pressure k. [Cyclopropane] = (0.25-10)% P(Total) = (0.5-7.0) atm.	EX 970-1265		1.58(15)	0	32713	1
74 BAR/COC ²⁾	EX 950		4.43			1
74 BAR/COC ²⁾	EX 1052		1.35(2)			1
74 BAR/COC ²⁾	EX 1096		8.73(2)			1
74 BAR/COC ²⁾	EX 1302		2.16(3)			1
74 BAR/COC ²⁾	EX 1452		5.96(3)			1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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74 BAR/COC ²⁾ EX 1653 2.34(4) 1

²⁾ k_a . M = He + Ar. Cyclopropane thermal isomerization behind reflected shock-waves in a single-pulse shock-tube. Limiting high-pressure k. Other rate constants at various temperatures within the 950-1653 K range are tabulated. The Arrhenius plot shows a pronounced curvature in the vicinity of 1080 K.

[Cyclopropane] = (0.2-1.0)%.

71 BRA/FRE ³⁾ EX 1060-1300 7.94(11) 0 27665 1

71 BRA/FRE ³⁾ EX 1350-1800 5.62(4) 0 5834 1

³⁾ k_{overall} . M = Ar. Shock-tube pyrolysis.
P(Total) = 500 torr.



(Racemic mixture)

Cyclopropane-1,2-d₂, (1S-trans)-

→ Cyclopropane-1,2-d₂, cis- (a)

→ Cyclopropane-1,2-d₂, trans-(±)- (racemic) (b)

76 BER/PED ¹⁾ EX 696 (6.75±0.14)(-5) 1

k_a . Thermal trans-cis isomerization.

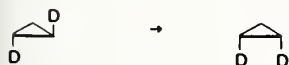
76 BER/PED ¹⁾ EX 696 (6.33±0.14)(-5) 1

k_b . Thermal racemization.

¹⁾ trans-(+)-Cyclopropane-1,2-d₂ thermal stereomutation. Gas-chromatography.

Supersedes 75 BER/PED.

P = 631 torr.



Cyclopropane-1,2-d₂, (1R-trans)-

→ Cyclopropane-1,2-d₂, cis-

76 BER/PED EX 696 (6.75±0.14)(-5) 1

Thermal trans-cis isomerization of optically active trans-(-)-Cyclopropane-1,2-d₂ in a reaction vessel. Gas-chromatography.

Supersedes 75 BER/PED.

P = 631 torr.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃CH₂CH₂ (+ M) → CH₃ + CH₂=CH₂ (+ M)						
Propyl						
71 PAP/LAI Limiting high-pressure k. M = CH ₃ CH ₂ CH ₃	EX	525-623	2.5(14)	0	16407±252	1
75 CAM/MAR	EX	676-813	1.26(12)	0	16359±962	1 3.16
80 GAW/MAK ¹⁾ At 228.8 nm.	EX	298	2.9(10)			1
80 GAW/MAK ¹⁾ At 253.7 nm.	EX	298	7.0(9)			1
¹⁾ H ₂ S irradiation with UV-light. Reaction of hot H atoms with Propene in a conventional vacuum system. Best data fit. P = (0.4-760) torr.						
71 PAP/LAI Limiting low-pressure k. M = CH ₃ CH ₂ CH ₃	EX	525-623	2.5(7)	0	8556±252	2
CH₃CH₂CH₂ + O₂ → CH₃CH=CH₂ + HO₂ (a)						
→ CH ₃ CH ₂ CHO + OH (b)						
→  + OH (c)						
→ CH ₃ CH ₂ CH ₂ O ₂ (d)						
Propyl + Oxygen molecule						
71 BAK/BAL ¹⁾ Least-squares treatment.	RL	753	(1.41±0.23)(6)			2/1
71 BAK/BAL ¹⁾ Computer treatment.	RL	753	(1.25±0.20)(6)			2/1
¹⁾ k _a /k _{ref} . k _{ref} : CH ₃ CH ₂ CH ₂ → CH ₃ + CH ₂ =CH ₂						
71 BAK/BAL k _a .	ES	753	3.8(10)			2
71 BAK/BAL k _b .	ES	753	1.1(8)			2
71 BAK/BAL k _c .	ES	753	3.1(9)			2
82 RUI k _d . M = N ₂ . Photoionization mass-spectrometry. k increases with the pressure. Near high-pressure limiting k. P(Total) = 4 torr.	EX	298	(3.43±0.10)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃CH₂CH₂ + O₃ → products						
Propyl + Ozone						
82 PAL Photoionization mass-spectrometry. Propyl formed by photodissociation of CH ₃ CH ₂ CH ₂ NO ₂ . P = 2 torr.	EX	298	(1.47±0.29)(13)			2
CH₃CH₂CH₂ + HCHO → CH₃CH₂CH₃ + CHO (a) → CH₃CH₂CH₂CH₂O (b)						
Propyl + Formaldehyde						
80 KNO/NAC ¹⁾ k _a .	RN	333-363	1.0(11)	0	3921±253	2 2.0
80 KNO/NAC ¹⁾ k _b .	RN	333-363	7.94(10)	0	3367±253	2 3.16
¹⁾ Azopropane/Formaldehyde photolysis. Mass-spectrometry.						
CH₃CH₂CH₂ + CH≡CH → cis-CH₃CH₂CH₂CH=CH[†] (a) → trans-CH₃CH₂CH₂CH=CH[†] (b)						
Propyl + Ethyne						
72 WAT/OLS k _a + k _b . Azo-n-propane photolysis. P = (90-480) torr.	ES	343-405	1.15(12)	0	4529	2
CH₃CH₂CH₂ + CH₂=CH₂ → CH₃CH₂CH₂CH₂CH₂[†]						
Propyl + Ethene						
71 WAT/LAW Azo-n-propane Photolysis. k determined relative to the reaction: CH ₃ CH ₂ CH ₂ + CH ₃ CH ₂ CH ₂ · → CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃	ES	330-373	1.41(11)	0	3724	2
CH₃CH₂CH₂ + CH₃CH₂CH₂ → CH₃CH=CH₂ + CH₃CH₂CH₃ (a) → CH₃CH₂CH₂CH₂CH₂CH₃ (b)						
Propyl						
71 FAL/SUN k _a /k _b .	RL	298	1.5(-1)			2/2
81 ADA/BAS1 ¹⁾ k _a .	EX	298	(1.9±0.2)(12)			2
81 ADA/BAS1 ¹⁾ k _b .	EX	298	(1.0±0.1)(12)			2
¹⁾ Azo-n-propane Flash-photolysis. Kinetic Spectroscopy.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{CH}_2\text{CH}_2 + (\text{CH}_3)_2\text{CH} \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_3$ (a) $\rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{CH}_3$ (b)							
Propyl + Ethyl, 1-Methyl- (i-Propyl)							
71 FAL/SUN k_a/k_b .	RL	298	4.1(-1)				2/2
$\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHO} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CO}$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CHCHO}$ (b) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CHCH}_2\text{CHO}$ (c)							
Propyl + Butanal							
79 FOE/BER ¹⁾ k_a .	DE	273-529	1.0(11)	0	3322±252	2	2.0
79 FOE/BER ¹⁾ k_b .	DE	273-529	3.98(10)	0	4328±352	2	3.16
79 FOE/BER ¹⁾ k_c .	DE	426-529	3.98(10)	0	5184	2	
¹⁾ Butanal photolysis. Rate constants determined relative to the reaction: $\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ on the basis of a suggested reaction scheme.							
$\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ $\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ (b) $\rightarrow \text{CH}_3(\text{CH}_2)_6\text{CH}_3$ (c)							
Propyl + Pentyl							
71 WAT/LAW ¹⁾ ($k_a + k_b + k_c$)/ k_c . Estimated ratio.	RL	330	1.14				2/2
71 WAT/LAW ¹⁾ k_b/k_c .	RL	330	5.6(-2)				2/2
¹⁾ Azo-n-propane Photolysis.							
$\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3$ $\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_3$ (b) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3$ (c) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{trans-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3$ (d) $\rightarrow (\text{CH}_3\text{CH}_2\text{CH}_2)_2\text{CH}(\text{CH}_3)$ (e)							
Propyl + Butyl, 1-methyl-							
71 WAT/LAW ($k_a + k_b + k_c + k_d + k_e$)/ k_e . Azo-n-propane Photolysis. Estimated ratio.	RL	330	1.41				2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$(\text{CH}_3)_2\text{CH} \rightarrow \text{H} + \text{CH}_3\text{CH}=\text{CH}_2$ (a)							
$\rightarrow \text{CH}_3 + \text{CH}_2=\text{CH}_2$ (b)							
Ethyl, 1-methyl- (i-Propyl)							
71 PAP/LAI	EX	525-623	2.0(14)	0	19480	1	
k_a . Limiting high-pressure k. M = $\text{CH}_3\text{CH}_2\text{CH}_3$.							
75 CAM/MAR	EX	676-813	2.51(13)	0	20569±1202	1	5.01
k_a .							
75 BUL/MAR	RL	667-770	4.0(-2)	0	0	1/1	
k_b/k_a .							
Static system pyrolysis. Average ratio.							
$(\text{CH}_3)_2\text{CH}^\dagger \rightarrow \text{H} + \text{CH}_3\text{CH}=\text{CH}_2$ (a)							
$\rightarrow \text{CH}_3 + \text{CH}_2=\text{CH}_2$ (b)							
Ethyl, 1-methyl- (-Propyl)							
72 ARI/STE ¹⁾	ES	2)	1.0(14)	0	20634	1	
k_a .							
72 ARI/STE ¹⁾	ES	2)	1.0(14)	0	23150	1	
k_b .							
¹⁾ $(\text{CH}_3)_2\text{CH}^\dagger$ formed by Photolysis of Azoisopropane.							
²⁾ Arrhenius expression determined from a pressure-wavelength data-fit to the RRKM theory.							
$(\text{CH}_3)_2\text{CH} + \text{O}_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{HO}_2$ (a)							
$\rightarrow (\text{CH}_3)_2\text{CHO}_2$ (b)							
Ethyl, 1-methyl- (i-Propyl) + Oxygen molecule							
76 BAL/CLE ¹⁾	RL	713	(3.06±0.25)(3)			2/2	
k_{ref} : $(\text{CH}_3)_3\text{CH} + \text{H}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{H}$							
76 BAL/CLE ¹⁾	RL	713	(7.68±0.30)(3)			2/2	
k_{ref} : $(\text{CH}_3)_3\text{CH} + \text{D}_2 \rightarrow \text{CH}_3\text{CHDCH}_3 + \text{D}$							
¹⁾ k_a/k_{ref} .							
82 RUI	EX	298	(7.83±1.20)(12)			2	
k_b . M = He. Photoionization Mass-spectrometry.							
Near high-pressure limiting k.							
k is P-independent.							
P(Total) = 1 torr.							
$(\text{CH}_3)_2\text{CH} + \text{O}_3 \rightarrow \text{products}$							
Ethyl, 1-methyl- (i-Propyl) + Ozone							
82 PAL	EX	298	(2.80±0.32)(13)			2	
Photoionization mass-spectrometry.							
$(\text{CH}_4)_2\text{CH}$ formed by photodissociation of							
$(\text{CH}_3)_2\text{CHNO}_2$.							
P = 2 torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_2\text{CH} + \text{H}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{H}$						
Ethyl, 1-methyl- (i-Propyl) + Hydrogen molecule						
76 BAL/CLE	RL	713	(2.51±0.20)			2/2
$k_{\text{ref}}:$						
$(\text{CH}_3)_2\text{CH} + \text{D}_2 \rightarrow \text{CH}_3\text{CHDCH}_3 + \text{D}$						
$(\text{CH}_3)_2\text{CH} + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CH}_2$						
Ethyl, 1-methyl- (i-Propyl) + Ethane						
74 SZI/MAR	RN	496-548	2.511(10)	0	6392±403	2 2.51
76 SZI/MAR	RN	496-548	1.0(11)	0	6495±361	2 2.51
Azoisopropane sensitized pyrolysis of Ethane in a static system. k determined relative to the reaction: $(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CH} \rightarrow (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$ P = (38-230) torr.						
$(\text{CH}_3)_2\text{CH} + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_2=\text{CHCH}_2$						
Ethyl, 1-methyl (i-Propyl) + 1-Propene						
76 SZI/MAR	RN	496-548	5.01(9)	0	3850±850	2 5.01
Azoisopropane sensitized pyrolysis of Ethane in a static system. k determined relative to the reaction: $(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CH} \rightarrow (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$ P = (38-230) torr.						
$(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CH} \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_3$ (a) $\rightarrow (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$ (b)						
Ethyl, 1-methyl- (i-Propyl)						
71 FAL/SUN ¹⁾	RL	298	6.9(-1)			2/2
72 ARI/STE ¹⁾	RL	295	(5.7±0.5)(-1)			2/2
Azoisopropane Photolysis.						
74 GOL/PIS ¹⁾	RL	683	(1.0±0.5)			2/2
74 GOL/PIS ¹⁾	RL	808	(1.5±0.5)			2/2
76 PAR/QUI ¹⁾	RL	298	(6.5±0.5)(-1)			2/2
77 MCK/TUR ¹⁾	RL	518	5.2(-1)			2/2
Azoisopropane thermolysis.						
77 MCK/TUR ¹⁾	RL	573	4.9(-1)			2/2
Azoisopropane thermolysis.						
79 KIR/PAR ¹⁾	RL	302	(6.0±0.1)(-1)			2/2
Photolysis of trans-2,2'-Azopropane. Gas-chromatography. Mass-spectrometry.						
79 SZI ¹⁾	RL	494-546	(7.6±1.6)(-1)			2/2
Azoisopropane pyrolysis in a static system. Average ratio.						
¹⁾ k_a/k_b .						

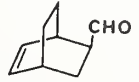
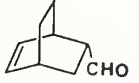
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/(ref), A, A/(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 ARR/KIR k _a . Molecular Modulation Spectrometer technique.	EX	301-424	(3.01±0.60)(12)	0	-25±313	2	
81 ADA/BAS1 k _a . Flash-photolysis of Azoisopropane. Kinetic spectroscopy.	EX	298	(5.0±1.2)(12)			2	
82 DEM/LES k _a + k _b . Flash-photolysis. Laser-resonance-absorption. (CH ₃) ₂ CH generated by flashing NH ₃ in presence of 1-Propene. Best data-fit.	ES	298	6.0(12)			2	
72 HIA/BEN1 ¹⁾	ES	415	3.98(11)			2	12.6
74 GOL/PIS ¹⁾	RN	683-808	3.16(12)	0	0	2	1.58
76 PAR/QUI ¹⁾	RN	298	(5.0±1.2)(12)			2	
78 ARR/KIR ¹⁾ Molecular Modulation Spectrometer technique.	EX	301-424	(8.43±1.69)(12)	0	161±313	2	
81 ADA/BAS1 ¹⁾ Flash-photolysis of Azoisopropane.	EX	298	(7.7±1.6)(12)			2	
¹⁾ k _b . (CH ₃) ₂ CH + (CH ₃) ₂ CHCHO → CH ₃ CH ₂ CH ₃ + (CH ₃) ₂ CHCO (a) → CH ₃ CH ₂ CH ₃ + (CH ₃) ₂ CCHO (b)							
Ethyl, 1-methyl- (i-Propyl) + Propanal, 2-methyl-							
76 BAL/CLE (k _a + k _b)/k _{ref} . k _{ref} : (CH ₃) ₂ CH + O ₂ → CH ₃ CH=CH ₂ + HO ₂	RL	713	3.2(-3)			2/2	1.1
(CH ₃) ₂ CH + (CH ₃) ₄ C → CH ₃ CH ₂ CH ₃ + (CH ₃) ₃ CCH ₂							
Ethyl, 1-methyl- (i-Propyl) + Propane, 2,2-dimethyl- (Neopentane)							
79 SZI/MAR Neopentane pyrolysis in presence of Azo- isopropane. P(Total) = (15-300) torr.	EX	512-571	3.16(10)	0	6616±601	2	6.31
(CH ₃) ₂ CH + (CH ₃) ₂ CHCH(CH ₃) ₂ → CH ₃ CH ₂ CH ₃ + (CH ₃) ₂ CHCH(CH ₃)CH ₂ (a) → CH ₃ CH ₂ CH ₃ + (CH ₃) ₂ CHC(CH ₃) ₂ (b)							
Ethyl, 1-methyl- (i-Propyl) + Butane, 2,3-dimethyl-							
75 BUL/MAR ¹⁾ (k _a + k _b)/k _{ref} . k _{ref} : (CH ₃) ₂ CH → H + CH ₃ CH=CH ₂	RL	667-770	6.31(-1)	0	-9863	2/1	
75 BUL/MAR ¹⁾ k _a + k _b . ¹⁾ Static system pyrolysis.	ES	667-770	1.58(13)	0	10710	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CHN}=\text{NCH}(\text{CH}_3)_2$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_2\text{CH}(\text{CH}_3)\text{N}=\text{NCH}(\text{CH}_3)_2$							
Ethyl, 1-methyl- (i-Propyl) + Diazene, bis(1-methylethyl)- (Azoisopropane)							
79 SZI Azoisopropane pyrolysis in a static system.	EX	494-546	5.01(9)	0	3248±241	2	1.58
$\text{CH}_3\text{CH}_2\text{CH}_3 (+\text{M}) \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}_2 (+\text{M})$ (a) $\rightarrow \text{any other products } (+\text{M})$ (b)							
Propane							
79 FRA/ROG2 k _a . M = Ar. Pyrolysis in a wall-less reactor. Average k at the mean experimental T. Other k values within (967-1051) K T-range also given. Approximate fitted values. P(Ar) = 600 torr.	EX	1008	(3.0±1.5)(-3)			1	
81 CHI/SKI1 ¹⁾ k _a . Experimental k.	EX	1200-1450	6.7(16)	0	45395	1	
81 CHI/SKI1 ¹⁾ k _a . Recommended k.	SE	1200-1450	2.5(16)	0	44036	1	2.0
¹⁾ Pyrolysis behind reflected shock-waves. Resonance-absorption spectroscopy. Same data given in 79 CHI/SKI. P (Total) = (2-3) atm.							
81 JUS/SCA k _a . Pyrolysis in a jet-stirred tank-reactor. Gas-chromatography. P(Propane) ~20 torr.	EX	873-1053	≈4.47(16)	0	≈42627	1	
82 ALA k _a . Pyrolysis behind incident shock-waves. Laser-schlieren. Limiting high-pressure k. P = (150-550) torr.	EX	1400-1800	7.74(11)	0	28048	1	
72 ILL/SZA ²⁾	EX	910-1075	6.37(13)	0	31807	1	1.1
74 BAK/NOV ²⁾	EX	973-1123	3.5(12)	0	28737±1007	1	
78 VER/BEL ²⁾ Pyrolysis in a flow-reactor. Average ratio. k _{ref} : $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{products}$.	RL	873-1103	(6.35±1.05)(-1)			1/1	
79 BRA ²⁾ Pyrolysis in a single-pulse shock-tube.	EX	1210-1680	1.98(8)	0	18885	1	1.38
79 ZYC/BAC ²⁾ Pyrolysis in a tubular reactor. P = 1 atm.	EX	1000-1120	1.7(11)	0	26572±352	1	
81 HAU/SAN ²⁾ Pyrolysis in a flow-reactor.	EX	1110-1235	3.16(12)	0	29517±906	1	2.19
²⁾ k _{overall} .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 CHI/SKI k_a . M = Ar. Pyrolysis behind reflected shock-waves. P = (2-3) Atm.	EX	1200-1450	2.6(21)	0	45244	2
82 ALA k_a . Pyrolysis behind incident shock-waves. Limiting low-pressure k. P = (150-550) torr.	EX	1800-2300	2.68(17)	0	28278	2
$\text{CH}_3\text{CH}_2\text{CH}_3^\dagger \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}_2$ (a) $\rightarrow \text{CH}_4 + \text{CH}_2=\text{CH}_2$ (b)						
Propane						
71 LEX/MAR1 ¹⁾ k_a . P(Ar) = (4-16) torr.	RL	290	(3.99±0.46)(-8)			1/2
72 GRO/HAS k_a .	EX	298	(4.7±1.2)(8)			1
71 LEX/MAR1 ¹⁾ k_b . P(Ar) = (4-16) torr.	RL	290	(3.22±0.28)(-8)			1/2
71 LEX/MAR2 ¹⁾ k_b . P(Ar) = (4-12) torr.	RL	290	(3.28±0.41)(-8)			1/2
¹⁾ M = Ar. Discharge flow. $\text{CH}_3\text{CH}_2\text{CH}_3^\dagger$ formed by $\text{H} + (\text{CH}_3)_2\text{CH}$. $k_{\text{ref}}: \text{CH}_3\text{CH}_2\text{CH}_3^\dagger + \text{M} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{M}$.						
$\text{CD}_3\text{CD}_2\text{CD}_3 \rightarrow \text{CD}_3 + \text{CD}_3\text{CD}_2$						
Propane-d ₈						
81 CHI/SKI1 ¹⁾	EX	1200-1450	6.7(16)	0	45395	1
81 CHI/SKI1 ¹⁾ Recommended k. ¹⁾ Pyrolysis behind reflected shock-waves. Resonance-absorption spectroscopy. Same data given in 79 CHI/SKI. P(Total) = (2-3) atm.	SE	1200-1450	2.5(16)	0	44036	1 2.0
$\text{CH}_2=\text{CHCHO} + $  $\rightarrow $  CHO (a)						
$\rightarrow $  CHO (b)						
2-Propenal (Acrolein) + 1,3-Cyclohexadiene $\rightarrow$ Bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, (1 α ,2 α ,4 α)- (Exo form) (a) $\rightarrow$ Bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, (1 α ,2 β ,4 α)- (Endo form) (b)						
76 HUY/PAT ¹⁾ k_a .	EX	486-871	3.24(5)	0	10382±25	2 1.05

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 HUY/PAT ¹⁾ k _b . ¹⁾ Diels-Alder addition of Acrolein to 1,3-Cyclohexadiene in a Pyrex reaction vessel. Gas-chromatography. P = (55-240) torr.	EX	486-871	4.47(5)	0	9799±25	2 1.05
 $\text{CH}_3\text{CH}_2\text{CO} (+\text{M}) \rightarrow \text{CH}_3\text{CH}_2 + \text{CO} (+\text{M})$ Propyl, 1-oxo-						
73 WAT/THO	ES	238-278	5.89(12)	0	7247	1
76 ERN/SPI M = Ar. Limiting high-pressure k. Supersedes 75 ERN/SPI.	EX	1350-1650	2.7(16)	0	41137±1443	1
 $\text{CH}_3\text{CH}_2\text{CO} + \text{O}_2 \rightarrow \text{CH}_2=\text{CH}_2 + \text{CO}_2 + \text{OH}$ Propyl, 1-oxo- + Oxygen molecule						
79 BAL/LEW1 M = N ₂ . Oxidation in an aged boric-acid-coated vessel. k _{ref} : $\text{CH}_3\text{CH}_2\text{CO} + \text{M} \rightarrow \text{CH}_3\text{CH}_2 + \text{CO} + \text{M}$	RL	713	(1.12±0.10)(-1)			2/2
 $\text{CH}_2=\text{CHCH}_2\text{O}_2 \rightarrow \text{CH}_2=\text{CHCH}_2 + \text{O}_2$ 2-Propenyldioxy						
81 RUI/BAY M = He. Photoionization mass-spectrometry. k ₁ Measured simultaneously with k ₋₁ . Allyl formed by Hexadiene/O ₂ flash-photolysis at 193 nm., with anArF excimer laser. P(1,5-Hexadiene) ~100 mtorr. P(O ₂) = (4.1-27.4) mtorr. P(Total) = 2.8 torr.	EX	348	(2.60±0.96)(1)			1
 $\text{CH}_3\text{CH}_2\text{CHO} + \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OOH} \rightarrow \text{products}$ Propanal + Propaneperoxoic acid						
74 DIX/SKI1	RN	337	1.0			2
 $\text{C}_4\text{H}_8\text{O} \rightarrow \text{HCHO} + \text{CH}_2=\text{CH}_2$ Oxetane						
75 HOL/SCO Pyrolysis in a cylindrical Pyrex vessel. High-vacuum system. Gas-chromatography. NMR, and IR-Spectrometry. P ₀ = (0.4-117) torr.	EX	693-753	5.13(15)	0	31719±422	1 2.04

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{H}_3\text{C}-\text{C}(\text{O})-\text{CH}_2$							
→ CH ₃ CH ₂ CHO (a)							
→ (CH ₃) ₂ CO (b)							
→ CH ₂ =CHCH ₂ OH (c)							
→ CH ₂ =CHOCH ₃ (d)							
Oxirane, methyl-							
77 FLO ¹⁾ k _a . P _O = 131 torr.	EX	654-717	2.45(14)	0	29434±289	1	1.51
77 FLO ¹⁾ k _b . P _O = 131 torr.	EX	654-717	1.51(14)	0	30131±289	1	1.51
77 FLO ¹⁾ k _b . Limiting high-pressure k. RRKM calculation.	ES	654-717	1.70(14)	0	30552	1	
77 FLO ¹⁾ k _c . P _O = 131 torr.	EX	654-717	7.94(12)	0	28760±241	1	1.41
77 FLO k _d . P _O = 131 torr.	EX	654-717	3.24(14)	0	29578±373	1	1.70
77 FLO ¹⁾ ²⁾ Without added NO.	EX	654-717	4.37(14)	0	29470±156	1	1.26
77 FLO ¹⁾ ²⁾ Packed reaction vessel without added NO.	EX	654-717	3.09(14)	0	29145±397	1	1.78
77 FLO ¹⁾ ²⁾ With 8.5% NO added.	EX	654-717	4.07(14)	0	29482±229	1	1.38
¹⁾ Thermolysis in a static system. Gas-chromatography. Mass-spectrometry. P = (5-326) torr.							
²⁾ k _a + k _b + k _c + k _d .							
HC(O)OCH ₂ CH ₃ → products Formic acid ethyl ester (Ethyl formate)							
71 BLA/SAN	EX	830-903	2.19(12)	0	24207±252	1	
CH ₃ C(O ¹⁸)OCH ₃ → CH ₃ COO ¹⁸ CH ₃ Acetic- ¹⁸ O acid ¹⁶ O-methyl ester							
81 CAR/EGS ¹⁾	EX	1253	3.72(2)			1	
81 CAR/EGS ¹⁾	EX	1404	1.78(3)			1	
¹⁾ Flash-vacuum thermolysis.							
CH ₃ C(O)OCH ₃ → products Acetic acid methyl ester (Methyl acetate)							
82 BLA/SHR Thermolysis. Apparent k, reflecting the importance of heterogeneous processes in the decomposition. P(Methyl acetate) ₀ = (30-70) torr.	EX	743-834	2.00(6)	0	17358±780	1	2.63

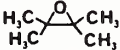
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{CH}_2\text{CH}_2\text{O} + \text{NO} \rightarrow \text{CH}_3\text{CH}_2\text{CHO} + \text{HNO}$ (a)							
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{ONO}$ (b)							
Propoxy + Nitrogen oxide (NO)							
80 ROS	RL	298	(1.1±0.1)(-1)				2/2
k_a/k_b . Propyl nitrite/NO ₂ photolysis at 366 nm.							
$\text{CH}_3\text{CH}_2\text{CH}_2\text{O} + \text{NO}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CHO} + \text{HONO}$ (a)							
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{ONO}_2$ (b)							
Propoxy + Nitrogen oxide (NO ₂)							
80 ROS	RL	298	(1.1±0.1)(-1)				2/2
k_a/k_b . Propyl nitrite photolysis at 366 nm. in presence of NO ₂ . Gas-chromatography.							
75 MEN/GOL	DE	300	3.16(12)	0	0	2	
k_b . Estimated from thermochemical data and the assumption that $E_a \sim 0$.							
77 BAR/BEN2	ES	580-800	3.16(12)			2	
k_b . VLP-Pyrolysis. RRKM best-fit estimate.							
$(\text{CH}_3)_2\text{CHO} \rightarrow \text{CH}_3\text{CHO} + \text{CH}_3$ (a)							
$\rightarrow (\text{CH}_3)_2\text{CO} + \text{H}$ (b)							
Ethoxy, 1-methyl-							
75 BAT/MCC	ES	393-473	2.51(14)	0	8606	1	
k_a .							
79 BAT ¹⁾	ES	393-473	3.98(14)	0	8656±503	1	3.16
k_a .							
79 BAT ¹⁾	ES	393-473	2.00(14)	0	10820	1	
k_b . Preliminary k.							
¹⁾ Static system.							
Same data given in 77 BAT/MIL1.							
$(\text{CH}_3)_2\text{CHO} + \text{NO} \rightarrow (\text{CH}_3)_2\text{CHONO}$ (a)							
$\rightarrow (\text{CH}_3)_2\text{CO} + \text{HNO}$ (b)							
$\rightarrow (\text{CH}_3)_2\text{CHONO}$ (c)							
Ethoxy, 1-methyl- + Nitrogen oxide (NO)							
74 BAT/MIL ¹⁾	ES	393-473	2.51(13)	0	0±503	2	2.51
77 BAT/MIL ¹⁾	ES	403-433	3.16(13)	0	0±403	2	2.51
¹⁾ k_a .							
74 BAT/MIL ²⁾	ES	393-473	3.98(12)	0	0±503	2	3.16
77 BAT/MIL ²⁾	ES	503-433	3.16(13)	0	0±503	2	2.51
²⁾ k_b .							
74 BAT/MIL	ES	393-473	2.51(13)	0	0±503	2	2.51
k_c .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_2\text{CHO} + (\text{CH}_3)_2\text{CHOOH} \rightarrow (\text{CH}_3)_2\text{CHO}_2 + (\text{CH}_3)_2\text{CHOH}$						
Ethoxy, 1-methyl- + Hydroperoxide, 1-methylethyl-						
79 KIR/PAR trans-2,2'-Azopropane photolysis. Mass-spectrometry. $k_{\text{ref}}: (\text{CH}_3)_2\text{CHO} + \text{O}_2 \rightarrow (\text{CH}_3)_2\text{CO} + \text{HO}_2$.	RL	302	(1.66±0.05)(-2)			2/2
$\text{CH}_3\text{CH}_2\text{CH}_2\text{O}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{O}_2$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{O} + \text{CH}_3\text{CH}_2\text{CH}_2\text{O} + \text{O}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{OH} + \text{CH}_3\text{CH}_2\text{CHO} + \text{O}_2$ (b)						
Propyldioxy						
82 ADA/BAS1 $k_a + k_b$. Azo-n-propane Flash-photolysis in Ar. $P(\text{Azo-n-propane}) = (4.5-10)$ torr. $P(\text{Pentane}) = (0-86)$ torr. $P(\text{O}_2) = (2.2-670)$ torr. $P(\text{Ar}) = (0-540)$ torr. $P(\text{N}_2) = (0-720)$ torr.	EX	298	(2.0±0.2)(8)			2
$(\text{CH}_3)_2\text{CHO}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{NO}_2$						
Ethyldioxy, 1-methyl- + Nitrogen oxide (NO)						
82 ADA/BAS2 Azoisopropane Flash-photolysis. Kinetic-spectroscopy. k is P-independent in the (55-400) torr. range. $P(\text{NO}_2) = (1.1-6.1) \times 10^{-2}$ torr. $P(\text{NO}) = (1.4-6.1) \times 10^{-2}$ torr. $P(\text{Azoisopropane}) \sim 2$ torr. $P(\text{O}_2) = (5.7-15.5)$ torr.	EX	298	(2.1±0.2)(12)			2
$(\text{CH}_3)_2\text{CHO}_2 + \text{NO}_2 \rightarrow (\text{CH}_3)_2\text{CHOONO}_2$						
Ethyldioxy, 1-methyl- + Nitrogen oxide (NO ₂)						
82 ADA/BAS2 Azoisopropane Flash-photolysis. Kinetic spectroscopy. k is P-independent in the (55-400) torr. range. $P(\text{NO}_2) = (1.1-6.1) \times 10^{-2}$ torr. $P(\text{NO}) = (1.4-6.1) \times 10^{-2}$ torr. $P(\text{Azoisopropane}) \sim 2$ torr. $P(\text{O}_2) = (5.7-15.5)$ torr.	EX	298	(3.4±0.1)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$(\text{CH}_3)_2\text{CHO}_2 + (\text{CH}_3)_2\text{CHO}_2$							
$\rightarrow (\text{CH}_3)_2\text{CHO} + (\text{CH}_3)_2\text{CHO} + \text{O}_2$ (a)							
$\rightarrow (\text{CH}_3)_2\text{CHOH} + (\text{CH}_3)_2\text{CO} + \text{O}_2$ (b)							
Ethylidioxy, 1-methyl-							
79 KIR/PAR k_a . trans-2,2'-Azopropane photolysis. Gas-chromatography. Mass-spectrometry.	EX	302	(2.99±0.20)(8)			2	
82 COW/WAD k_a . trans-2,2'-Azopropane Photooxidation, with or without O_2 . $P(\text{O}_2) = (0-500)$ torr. $P(\text{trans-2,2'-Azoisopropane}) = 5$ torr. $P(\text{N}_2) = (300-500)$ torr.	EX	333-373	(1.38±0.26)(12)	0	2562±180	2	
79 KIR/PAR k_b . trans-2,2'-Azopropane photolysis. Gas-chromatography. Mass-spectrometry.	EX	302	(2.15±0.10)(8)			2	
82 COW/WAD k_b . trans-2,2'-Azopropane Photooxidation, with or without O_2 . $P(\text{O}_2) = (0-500)$ torr. $P(\text{trans-2,2'-Azoisopropane}) = 5$ torr. $P(\text{N}_2) = (300-500)$ torr.	EX	333-373	(2.44±0.31)(10)	0	1443±120	2	
78 KIR/PAR $k_a + k_b$. Azoisopropane/ O_2/N_2 photolysis.	EX	300-373	(1.43±0.10)(12)	0	2243±60	2	
82 ADA/BAS1 $k_a + k_b$. Azoisopropane flash-photolysis at 260 nm. in Ar. $P(\text{Azoisopropane}) = (4.5-10)$ torr. $P(\text{N}_2) = (0-720)$ torr. $P(\text{Ar}) = (0-540)$ torr. $P(\text{Pentane}) = (0-86)$ torr. $P(\text{O}_2) = (2.2-670)$ torr.	EX	298	(7.8±2.2)(8)			2	
$(\text{CH}_3)_2\text{CHO}_2 + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$							
$\rightarrow (\text{CH}_3)_2\text{CHO} +$ 							
Ethylidioxy, 1-methyl- + 2-Butene, 2,3-dimethyl-							
82 SWA/WAD Reaction of Isopropylperoxyl with 2,3-Dimethyl-2-butene in a Pyrex vessel. The radicals generated by trans-2,2'-Azopropane/ O_2/N_2 photooxidation. $P(2,3\text{-Dimethyl-2-butene}) = 20$ torr. $P(\text{trans-2,2'-Azoisopropane}) = 5$ torr. $P(\text{O}_2) = (50-450)$ torr. $P(\text{N}_2) = (25-450)$ torr.	EX	303-363	9.12(10)	0	4916±214	2	3.16

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
$(\text{CH}_3)_2\text{CHO}_2 + (\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2 \rightarrow \text{products}$						
Ethyldioxy, 1-methyl- + Propyldioxy, 1,1,2-trimethyl-						
75 ALC/MIL	ES	373	6.2(11)			2
$\text{CH}_3\text{CH}_2\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{CH}_2\text{CHO} + \text{H}_2$ (a)						
$\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{H}_2\text{O}$ (b)						
$\rightarrow \text{CH}_3 + \text{CH}_2\text{CH}_2\text{OH}$ (c)						
1-Propanol						
71 GON/LEW	EX	753-833	6.80(5)	0	13265	1
$k_a + k_b$.						
76 TSA1	ES	1080-1165	1.58(16)	0	41100	1
k_c .						
$(\text{CH}_3)_2\text{CHOH} \rightarrow (\text{CH}_3)_2\text{CO} + \text{H}_2$ (a)						
$\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{H}_2\text{O}$ (b)						
$\rightarrow \text{CH}_3 + \text{CH}_3\text{CHOH}$ (c)						
2-Propanol						
71 GON/LEW	EX	753-833	1.05(5)	0	12582	1
$k_a + k_b$.						
75 TRE	EX	721-801	1.0(14)	0	29039±1007	1 3.98
k_a .						
75 TRE	EX	721-801	1.26(13)	0	29290±1812	1 10.0
k_b .						
76 TSA1	ES	1080-1165	3.16(16)	0	41100	1
k_c .						
$\text{C}_3\text{H}_8\text{S} \rightarrow \text{HC}_2\text{S} + \text{CH}_2=\text{CH}_2$						
Thietane (Trimethylene sulfide)						
$\rightarrow \text{Methanethial} + \text{Ethene}$						
73 JEF/DAS	EX	980-1040	1.0(13)	0	24258	1
M = Ar.						
Thiethane thermolysis in a single-pulse shock-tube.						
$P_0 = (120-200) \text{ torr.}$						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃C(S)OCH₃ → CH₃(O)SCH₃						
Ethanethioic acid O-methyl ester						
72 OEL/TIN Thermal isomerization. T-range not given.	ES		~2.00(13)	0	23402	1
75 BIG/GAB ¹⁾	EX	629	8.97(-4)			2
75 BIG/GAB ¹⁾	EX	678-704	7.94(12)	0	23050	1
¹⁾ Thermal isomerization. Flow reactor pyrolysis.						
 						
Thietane, 1,1-dioxide- (Trimethylenesulfone)						
→ Cyclopropane + Sulfur dioxide						
75 COR/TSA Pyrolysis in a flow-tube reactor.	EX	638-678	1.26(16)	0	28100±500	1 2.0
 CH₂=CHCN + NH₂CH₂CH₂CN → NH(CH₂CH₂CN)₂						
2-Propenenitrile (Acrylonitrile)						
+ Propanenitrile, 3-amino- (β-Aminopropionitrile)						
→ Propanenitrile, 3,3'-iminobis-						
(β,β'-Iminodipropionitrile)						
82 SAI/MIC Reaction of 2-Propenenitrile with β-Amino- propionitrile in an Autoclave.	EX	303-408	7.43(10)	0	6241	2
 CH₃CH₂CN → CH₃ + CH₂CN (a)						
→ CH ₂ =CH ₂ + HCN (b)						
→ CH ₂ =CHCN + H ₂ (c)						
Propanenitrile						
78 KIN/GOD ¹⁾ k _a . In presence of excess C ₆ H ₅ NH ₂ .	EX	896-1020	1.77(15)	0	40764	1
73 DAS/EMO k _b .	EX	803-943	1.29(13)	0	34967±201	1 1.02
78 KIN/GOD ¹⁾ k _b . In absence of additives.	EX	896-1020	2.00(14)	0	34125±806	1 2.51

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 KIN/GOD ¹⁾ k _c . In absence of additives.	EX	896-1020	1.26(12)	0	29746±710	1	2.0
¹⁾ Pyrolysis in a flow-reactor. Gas-chromatography. [CH ₃ CH ₂ CN] ~ 6.0x10 ¹⁶ molec.cm ⁻³ . P ~ 760 torr.							
$\triangle_{\text{NH}_2} \rightarrow (\text{CH}_3\text{CH}=\text{CHNH}_2 = \text{CH}_3\text{CH}_2\text{CH}=\text{NH})$							
Cyclopropanamine							
→ (1-Propen-1-amine = 1-Propanimine)							
73 PAR/ROB Thermal isomerization in a silica reaction vessel with Pyrex vacuum-system. Gas-chro- matography. The intermediate product reacts with another molecule of reactant to form one molecule of:	EX	629-698	1.15(15)	0	29109±313	1	2.57
$\triangle_{\text{N}=\text{CHCH}_2\text{CH}_2}$							
(Cyclopropanamine, N-propylidene-).							
P ₀ = (15-60) torr.							
(CH ₃) ₂ CHONO → (CH ₃) ₂ CO + HNO (a) → CH ₃ CH=CH ₂ + HONO (b) → (CH ₃) ₂ CHO + NO (c)							
Nitrous acid 1-methylethyl ester (Isopropyl nitrite)							
75 BAT/MCC k _a .	ES	393-473	1.26(9)	0	13437	1	
77 BAT/MIL1 k _a .	ES	403-433	2.51(9)	0	13588	1	
78 BAT/ISL2 ¹⁾ k _a .	EX	433-473	2.00(14)	0	19577±503	1	3.16
78 BAT/ISL2 ¹⁾ k _b .	EX	433-473	5.01(12)	0	19074	1	
¹⁾ Pyrolysis in a static system.							
Gas-liquid chromatography.							
77 BAT/MIL1 k _c . Same data given in 74 BAT/MIL and 75 BAT/MCC.	ES	403-433	1.58(16)	0	20634±403	1	2.51

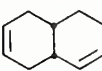
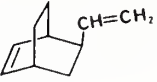
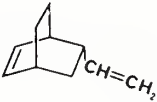
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{NHC(O)OCH}_3 \rightarrow \text{CH}_3\text{NCO} + \text{CH}_3\text{OH}$						
Carbamic acid, methyl-, methyl ester						
72 DAL/ZIO1 Thermolysis.	EX	643-695	2.45(12)	0	24187	1
$\text{CH}_3\text{CH}_2\text{CH}_2\text{ONO}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{O} + \text{NO}_2$						
Nitric acid propyl ester (n-Propyl nitrate)						
75 MEN/GOL RRKM fit of experimental data.	CO	300	3.15(16)	0	20131	1
77 BAR/BEN2 VLP-pyrolysis. RRKM best-fit estimate.	EX	580-800	3.16(16)	0	20131	1
$\text{CH}\equiv\text{CC}\equiv\text{C} \rightarrow \text{C}\equiv\text{CC}\equiv\text{C} + \text{H}$						
1,3-Butadiynyl						
80 FRA/JUS Thermolysis of Ethyne and 1,3-Butadiyne in Ar, behind shock-waves. Data-fit on the basis of a proposed mechanism. Total Conc. = $(0.4-1.6)\times 10^{19}$ molec.cm ⁻³ .	ES	2100-2300	$(1.35\pm 0.85)(14)$	0	58700	1
$\text{CH}\equiv\text{CC}\equiv\text{C} + \text{CH}\equiv\text{CC}\equiv\text{CH} \rightarrow \text{CH}\equiv\text{CC}\equiv\text{CC}\equiv\text{CC}\equiv\text{CH} + \text{H}$						
1,3-Butadiynyl + 1,3-Butadiyne						
80 FRA/JUS Thermolysis of Ethyne and 1,3-Butadiyne in Ar, behind shock-waves. Data-fit on the basis of a proposed mechanism. Total Conc. = $(0.4-1.6)\times 10^{19}$ molec.cm ⁻³ .	ES	1850-2300	$(3.5\pm 2.0)(13)$	0	0	2
$\text{CH}\equiv\text{CC}\equiv\text{CH} \rightarrow \text{CH}\equiv\text{CC}\equiv\text{C} + \text{H}$						
1,3-Butadiyne						
80 FRA/JUS Thermolysis of Ethyne and 1,3-Butadiyne in Ar, behind shock-waves. Total Conc. = $(0.4-1.6)\times 10^{19}$ molec.cm ⁻³ .	ES	1850-2300	$(2.2\pm 0.6)(14)$	0	58700±700	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$\text{CH}_3\text{CH}_2\text{C}\equiv\text{CH} \rightarrow \text{CH}_3 + \text{CH}_2\text{C}\equiv\text{CH}$							
1-Butyne							
78 KIN VLP-pyrolysis.	EX	1052-1152	3.16(15)	0	37343±1007	1	2.0
82 TRE/WRI Pyrolysis of 1-Butyne in a cylindrical silica reaction vessel with static system. Gas-chromatography. P = (50-1200) torr.	EX	652-731	1.58(17)	0	37645±1057	1	5.01
$\text{CH}_3\text{CH}_2\text{C}\equiv\text{CH} + \text{CH}_3\text{CH}_2\text{C}\equiv\text{CH} \rightarrow \text{CH}_3\text{CH}_2\text{C}=\text{CH}_2 + \text{CH}_3\text{CHC}\equiv\text{CH}$							
1-Butyne							
82 TRE/WRI Rate determining step. $\text{CH}_3\text{CH}_2\text{C}=\text{CH}_2$ decomposes further to give CH_3 and $\text{CH}_2=\text{C}=\text{CH}_2$. Pyrolysis of 1-Butyne in a cylindrical silica reaction vessel with static system. Gas-chromatography. P = (50-1200) torr.	EX	652-731	2.00(14)	0	24056±302	2	1.58
$\text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CH}_2=\text{CHCH}=\text{CH}_2$							
→  (a)							
→  (b)							
1,3-Butadiene							
77 HUY/LUY ¹⁾ k_a .	EX	464-557	4.47(10)	0	14313±50	2	1.10
77 HUY/LUY ¹⁾ k_b .	EX	464-557	8.91(9)	0	12345±60	2	1.12
¹⁾ Thermal reaction of 1,3-Butadiene in a static system. Gas-chromatography. P = (49-450) torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2=\text{CHCH}=\text{CH}_2 + $ 						
$\rightarrow $ 	(a)					
$\rightarrow $ 	(b)					
$\rightarrow $ 	(c)					
$\rightarrow $ 	(d)					
1,3-Butadiene + 1,3-Cyclohexadiene						
$\rightarrow $ Bicyclo[4.2.2]deca-3,7-diene	(a)					
$\rightarrow $ Naphthalene, 1,2,4a,5,8,8a-hexahydro-, cis-	(b)					
$\rightarrow $ Bicyclo[2.2.2]oct-2-ene, 5-ethenyl- (1 α ,4 α ,5 α)- (exo form)	(c)					
$\rightarrow $ Bicyclo[2.2.2]oct-2-ene, 5-ethenyl- (1 α ,4 α ,5 β)- (endo form)	(d)					
82 HUY/HUB2 ¹⁾ k _a .	EX	437-526	4.07(9)	0	12849±25	2 1.05
82 HUY/HUB2 ¹⁾ k _b .	EX	437-526	1.05(10)	0	12768±35	2 1.07
82 HUY/HUB2 ¹⁾ k _c .	EX	437-526	1.055(10)	0	13468±25	2 1.05
82 HUY/HUB2 ¹⁾ k _d .	EX	437-526	3.80(9)	0	12501±25	2 1.05
¹⁾ Thermal Diels-Alder addition in a static system. Gas-chromatography. P(1,3-Cyclohexadiene) = (50-93) torr. P(1,3-Butadiene) = (61-397) torr.						
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}^\dagger \rightarrow \text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2^\dagger$						
1-Butenyl $\rightarrow$ 3-Butenyl						
76 IBU/TSU ¹⁾	EX	348	1.00(9)			1
76 IBU/TSU ¹⁾	EX	396	1.05(9)			1
¹⁾ Photolysis of 3-Pentanone. $\text{CH}_3\text{CH}_2\text{CH}=\text{CH}^\dagger$ formed by $\text{CH}_3\text{CH}_2 + \text{CH}=\text{CH}$.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}=\text{CHCH}_2 + \text{H}_2\text{S} \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{SH}$ 2-Butenyl + Hydrogen sulfide						
80 RIC/BOI Static system. cis/trans-Butenyl equilibrium.	ES	750-816	1.0(14)	0	4680	2
$\text{CH}_3\text{CH}=\text{CHCH}_2 + \text{cis-CH}_3\text{CH}=\text{CHCH}_3$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}=\text{CHCH}_2$ 2-Butenyl + 2-Butene, (Z)-						
80 RIC/BOI ¹⁾ $k_{\text{ref}}: \text{CH}_3\text{CH}=\text{CHCH}_2 + \text{H}_2\text{S} \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{SH}$	RL	750-816	4.0(-1)	0	3271±503	2/2
80 RIC/BOI ¹⁾ ¹⁾ Static system. cis/trans-Butenyl equilibrium.	ES	750-816	≈3.98(13)	0	7952	2
$\text{trans-CH}_3\text{CH}=\text{CHCH}_2 \rightarrow \text{cis-CH}_3\text{CH}=\text{CHCH}_2$ 2-Butenyl, (E)-						
72 GOR/WAL $k_{\text{ref}}: \text{trans-CH}_3\text{CH}=\text{CHCH}_2 + \text{HI}$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{I}$ (a) $\rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}_3 + \text{I}$ (b)	RL	363	(1.64±0.28)(-6)			1/2
72 GOR/WAL	ES	363	5.01(4)			1
$\text{CH}_2=\text{CHCH}_2\text{CH}_2^\dagger \rightarrow [\text{CH}_3\text{CHCH}=\text{CH}_2^\dagger = \text{CH}_3\text{CH}=\text{CHCH}_2^\dagger]$ 3-Butenyl $\rightarrow$ [2-Propenyl, 1-methyl- = 2-Butenyl]						
76 IBU/TSU ¹⁾	EX	348	3.47(7)			1
76 IBU/TSU ¹⁾ ¹⁾ Photolysis of 3-Pentanone. $\text{CH}_2=\text{CHCH}_2\text{CH}_2^\dagger$ formed by isomerization of $\text{CH}_3\text{CH}_2\text{CH}=\text{CH}^\dagger$, which (in its turn) was formed by $\text{CH}_3\text{CH}_2 + \text{CH}=\text{CH}$.	EX	396	6.20(7)			1
$\text{CH}_2=\text{CHCH}_2\text{CH}_2 + \square^\bullet$ $\rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 + \square$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \square$ (b) $\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ $\square$ (c)						
3-Butenyl + Cyclobutyl 75 STE/RAB ¹⁾ k_a/k_c	RL	298	(1.3±0.5)(-1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 STE/RAB ¹⁾ k _b /k _c .	RL	298	(3.0±0.9)(-1)			2/2
75 STE/RAB ¹⁾ (k _a + k _b)/k _c .	RL	298	(4.3±0.7)(-1)			2/2
¹⁾ Disproportionation-combination ratios.						
CH ₃ C=CHCH ₃ [†] → CH ₃ C≡CH + CH ₃ (a) → CH ₃ C=CCH ₃ + H (b)						
1-Propenyl, 1-methyl- → 1-Propyne + Methyl (a) → 2-Butyne + Hydrogen atom (b)						
77 DIA/DOE ¹⁾ k _a /k _{ref} .	RL	298	(3.70±1.02)			1/1
77 DIA/DOE ¹⁾ k _b /k _{ref} .	RL	298	5.04			1/1
¹⁾ Study of the UV-photolysis of 1,2-Butadiene. CH ₃ C=CHCH ₃ [†] formed by H + CH ₃ =C=CH ₂ . k _{ref} : CH ₂ =CCH ₂ CH ₃ [†] → CH ₂ =C=CH ₂ + CH ₃						
CH ₂ =CHCHCH ₃ [†] → CH ₂ =CHCH=CH ₂ + H						
2-Propenyl, 1-methyl- (1-Methylallyl) → 1,3-Butadiene + Hydrogen atom						
77 DIA/DOE k/k _{ref} . Study of the UV-photolysis of 1,2-Butadiene. CH ₂ =CHCHCH ₃ [†] formed by H + CH ₃ =C=CH ₂ . k _{ref} : CH ₂ =CCH ₂ CH ₃ [†] → CH ₂ =C=CH ₂ + CH ₃	RL	298	(1.86±0.01)			1/1
trans-CH ₃ CHCH=CH ₂ → cis-CH ₃ CHCH=CH ₂						
2-Propenyl, 1-methyl-, (E)- (trans-1-Methylallyl)						
72 GOR/WAL	ES	363	5.0(4)			1
CH ₂ =CHCHCH ₃ + CH ₂ =CHCHCH ₃ → CH ₂ =CHCH(CH ₃)CH(CH ₃)CH=CH ₂						
2-Propenyl, 1-methyl- (1-Methylallyl)						
78 BAY 3-Methyl-1-butene, cis-2-Pentene, 1-Butene and trans-2-Butene Flash-photolysis. Kinetic Spectroscopy. Gas-chromatography.	EX	295	(3.5±0.4)(13)			2
CH ₂ C(CH ₃)=CH ₂ → CH ₂ =C=CH ₂ + CH ₃						
2-Propenyl, 2-methyl- (2-Methylallyl)						
73 TSA2 1050 K given by the author as central-T.	EX	996-1180	2.14(13)	0	25200±400	1 1.58

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2 + \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2$ $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$						
2-Propenyl, 2-methyl- (2-Methylallyl)						
73 BAY/BRO	EX	295	(2.6±0.3)(13)			2
73 TSA2	ES	996-1180	5.01(12)			2 3.98
1020 K given by the author as central-T.						
76 BAY	EX	295	(2.6±0.3)(13)			2
2-methyl-1-butene and 2-methyl-1-propene						
Kinetic Spectroscopy.						
Flash-Photolysis.						
$\square^\bullet + \square^\bullet \rightarrow \square + \square$ (a)						
$\rightarrow \text{cyclobutane}$ (b)						
Cyclobutyl						
75 STE/RAB	RL	298	(1.33±0.10)			2/2
k_a/k_b .						
Disproportionation-combination ratio.						
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3 + \text{CH}_2\text{CH}=\text{CH}_2$ (a)						
$\rightarrow$ any other products (b)						
1-Butene						
81 AYR/BAC	RL	750	6.31(-1)	0	2214	1/2
k_a/k_{ref} .						
Pyrolysis in a static system.						
$k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_2=\text{CH} + \text{CH}_3\text{CH}_2$						
73 SHI/KIN2	EX	829-1040	1.26(13)	0	29963	1
k_{overall} .						
$\text{cis-CH}_3\text{CH}=\text{CHCH}_3 (+\text{M}) \rightarrow \text{CH}_3\text{CH}=\text{CHCH}_2 + \text{H} (+\text{M})$ (a)						
$\rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{H}_2 (+\text{M})$ (b)						
$\rightarrow \text{CH}_2=\text{CHCH}_2 + \text{CH}_3 (+\text{M})$ (c)						
$\rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}_3 (+\text{M})$ (d)						
2-Butene, (Z)-						
80 RIC/BOI	ES	750-816	≈3.16(15)	0	43030	1
k_a .						
Conventional static system.						
Mass-spectrometry.						
73 ALF/GOL	DE	1100-1300	1.0(13)	0	32713±1007	1 3.98
k_b .						
RRKM fit of experimental data.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 MAS/RIC k _b . Static system. Same data given in 76 RIC/MAR. P ₀ ~ 50 torr.	EX	480-550	1.0(13)	0	32964±1007	1 3.16
74 JEF/BAU k _c . Average k.	RN	1150-1325	1.0(16)	0	40262	1
74 JEF k _d . Shock-tube cis-trans isomerization.	EX	990-1300	2.51(14)	0	33317	1 1.58
76 MAS/RIC k _d . Static system. Limiting high-pressure k. P ₀ = ~ 50 torr. Same data given in 76 RIC/MAR.	EX	753-823	3.98(13)	0	31203±503	1 2.0
73 COX k _d . M = SO ₂ (³ B ₁). 59% trans isomer formed.	RN	296	(1.62±0.08)(14)			2
74 SPR/AKI k _d . M = NO ₂ .	EX	298-366	7.26(10)	0	5944±42	2 1.14
cis-CH ₃ CH=CHCH ₃ + H ₂ S → CH ₃ CH ₂ CHCH ₃ + SH 2-Butene, (Z)- + Hydrogen sulfide						
80 RIC/BOI ¹⁾ k _{ref} : cis-CH ₃ CH=CHCH ₃ → CH ₃ CH=CHCH ₂ + H	ES	750-816	1.29(-2)	0	16004	2/1
80 RIC/BOI ¹⁾ ¹⁾ Static system. Mass-spectrometry.	ES	750-816	3.98(13)	0	27026	2
trans-CH ₃ CH=CHCH ₃ (+ M) → CH ₃ + CH ₂ =CHCH ₂ (+ M) (a) → cis-CH ₃ CH=CHCH ₃ (+ M) (b)						
2-Butene, (E)-						
74 JEF/BAU k _a . Average k.	EX	1150-1325	1.0(16)	0	40262	1
73 COX k _b . M = SO ₂ (³ B ₁). 41% cis isomer formed.	EX	296	(1.42±0.09)(14)			2
74 SPR/AKI k _b . M = NO ₂ .	EX	297-370	4.49(10)	0	6135±59	2 1.21
(CH ₃) ₂ C=CH ₂ → CH ₃ + CH ₂ CH=CH ₂ (a) → any other products (b)						
1-Propene, 2-methyl-						
76 BRA/WES2 k _a . Optimization by computer simulation on the basis of a proposed mechanism.	DE	1055-1325	1.82(18)	0	45107	1 1.23

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
74 BAK/NOV k_{overall} .	EX	973-1123	1.14(16)	0	38752±1258	1	
71 KOR/KAL k_{overall} . Pyrolysis in a quartz reactor. Gas-chromatography. P(Total) = 100 torr.	EX	1070-1200	1.89(16)	0	3976	1	1.2
$\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 \rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{CH}_2$ (a)							
$\rightarrow \square$ (b)							
1,4-Butanediyl $\rightarrow$ Ethene + Ethene (a)							
$\rightarrow$ Cyclobutane (b)							
72 BEA/GOL1 ¹⁾ k_a .	ES	969-1280	1.17(13)	0	4152	1	
72 BEA/GOL1 ¹⁾ k_b .	ES	969-1280	2.0(12)	0	3320	1	
¹⁾ Cyclobutane/Ar VLP-Pyrolysis. Mass-spectrometry.							
$\square \rightarrow \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ (a)							
$\rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{CH}_2$ (overall) (b)							
Cyclobutane $\rightarrow$ 1,4-Butanediyl (a)							
$\rightarrow$ Ethene + Ethene (b)							
72 BEA/GOL1 ¹⁾ k_a .	ES	969-1280	3.63(15)	0	31877	1	
72 BEA/GOL1 ¹⁾ k_b . Least squares treatment. RRKM data-fit.	EX	969-1280	2.63(15)	0	31203	1	
72 BEA/GOL1 ¹⁾ k_b . Best value based on the present experiments and all previously reported data.	SE	969-1280	3.16(16)	0	32969	1	
¹⁾ Cyclobutane/Ar VLP-Pyrolysis. Mass-spectrometry. Extrapolated limiting high-pressure k's.							
74 BAR/COC ²⁾	EX	891	6.03				1
74 BAR/COC ²⁾	EX	955	6.13(1)				1
74 BAR/COC ²⁾	EX	1000	1.26(2)				1
74 BAR/COC ²⁾	EX	1231	4.38(3)				1
74 BAR/COC ²⁾	EX	1400	1.13(4)				1
²⁾ k_b . M = Ar. Cyclobutane thermolysis behind reflected shock-waves in a single-pulse shock-tube.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
[Cyclobutane] = (0.2-1.0)%. Limiting high-pressure k. Other rate constants at various temperatures within the 891-1400 K range are tabulated. The Arrhenius plot shows a pronounced curvature in the vicinity of 1080 K.						
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_2=\text{CH}_2$						
Butyl						
80 GAW/GIE ¹⁾ At 313 nm. Experimental data-fit by using the Stern-Volmer equation.	EX	298	3.2(9)			1
80 GAW/GIE ¹⁾ At 313 nm. RRKM calculation.	CO	298	3.1(9)			1
80 GAW/GIE ¹⁾ At 334 nm. Experimental data-fit by using the Stern-Volmer equation.	EX	298	1.2(9)			1
80 GAW/GIE ¹⁾ At 334 nm. RRKM calculation.	CO	298	1.05(9)			1
¹⁾ HI irradiation with UV-light. Reaction of hot H atoms with 1-Butene in a Pyrex vacuum-system. P = (0.4-400) torr.						
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 + \text{O}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{HO}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{O}_2$ (b)						
Butyl + Oxygen molecule						
71 BAK/BAL k_a/k_{ref} . $k_{\text{ref}}: \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}=\text{CH}_2$	ES	753	1.57(6)			2/1
71 BAK/BAL k_a .	ES	753	2.8(11)			2
80 LEN/MCD k_b . M = He. 1-Iodobutane flash-photolysis. Photoionization Mass-spectrometer. Limiting high-pressure k. P-independent for (1-4) Torr range.	EX	298	(4.52±0.84)(12)			2
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (b)						
Butyl						
71 FAL/SUN k_a/k_b .	RL	298	1.4(-1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)$						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ (a)						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (b)						
Butyl + Propyl, 1-methyl-						
71 FAL/SUN	RL	298	4.5(-1)			2/2
k_a/k_b .						
$\text{CH}_3\text{CH}_2\text{CHCH}_3 \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}=\text{CH}_2$						
Propyl, 1-methyl-						
80 GAW/GIE ¹⁾	EX	298	2.5(9)			1
At 313 nm. Stern-Volmer experimental data-fit.						
80 GAW/GIE ¹⁾	CO	298	2.58(9)			1
At 313 nm. RRKM calculation.						
80 GAW/GIE ¹⁾	EX	298	1.05(9)			1
At 334 nm. Experimental data-fit by using the Stern-Volmer equation.						
80 GAW/GIE ¹⁾	CO	298	9.14(8)			1
At 334 nm. RRKM calculation.						
¹⁾ HI irradiation with UV-light. Reaction of hot H atoms with 1-Butene in a Pyrex vacuum system. P = (0.4-400) torr.						
$\text{CH}_3\text{CH}_2\text{CHCH}_3 + \text{O}_2 \rightarrow \text{cis-CH}_3\text{CH}=\text{CHCH}_3 + \text{HO}_2$ (a)						
$\rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}_3 + \text{HO}_2$ (b)						
$\rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_3 + \text{OH}$ (c)						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{OO}\cdot)\text{CH}_3$ (d)						
Propyl, 1-methyl- + Oxygen molecule						
71 BAK/BAL ¹⁾	RL	753	5.40(5)			2/1
k_a/k_{ref} .						
71 BAK/BAL ¹⁾	RL	753	9.63(5)			2/1
k_b/k_{ref} .						
¹⁾ $k_{\text{ref}}: \text{CH}_3\text{CH}_2\text{CHCH}_3 \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}=\text{CH}_2$						
71 BAK/BAL	ES	753	1.2(11)			2
k_a .						
71 BAK/BAL	ES	753	2.1(11)			2
k_b .						
71 BAK/BAL	ES	753	2.3(11)			2
k_c .						
80 LEN/MCD	EX	298	(1.00±0.13)(13)			2
k_d . M = He. 2-Iodobutane flash-photolysis. Photoionization Mass-spectrometer. Limiting high-pressure k. P-independent for (1-4) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃CH₂CHCH₃ + CH₃CH₂CHCH₃							
→ CH ₃ CH ₂ CH=CH ₂ + CH ₃ CH ₂ CH ₂ CH ₃ (a)							
→ cis-CH ₃ CH=CHCH ₃ + CH ₃ CH ₂ CH ₂ CH ₃ (b)							
→ trans-CH ₃ CH=CHCH ₃ + CH ₃ CH ₂ CH ₂ CH ₃ (c)							
→ CH ₃ CH ₂ CH(CH ₃)CH(CH ₃)H ₂ CH ₃ (d)							
Propyl, 1-methyl-							
71 FAL/SUN k _a /k _d .	RL	298	(4.1±0.2)(-1)				2/2
71 FAL/SUN (k _b + k _c)/k _d .	RL	298	(3.6±0.3)(-1)				2/2
71 FAL/SUN (k _a + k _b + k _c)/k _d .	RL	298	(7.7±0.5)(-1)				2/2
(CH₃)₂CHCH₂ + O₂ → (CH₃)₂C=CH₂ + HO₂ (a) → (CH₃)₂CHCHO + OH (b)							
Propyl, 2-methyl- + Oxygen molecule							
71 BAK/BAL ¹⁾	ES	753	8.92(5)				2/1
78 BAK/BAL ^{1) 3)} ¹⁾ k _a /k _{ref} . k _{ref} : (CH ₃) ₂ CHCH ₂ → CH ₃ + CH ₃ CH=CH ₂	RL	753	(7.75±1.00)(5)				2/1
71 BAK/BAL ²⁾	ES	753	2.3(10)				2
78 BAK/BAL ^{2) 3)}	RN	753	(6.8±3.4)(10)				2
78 BAK/BAL ^{2) 3)} ²⁾ k _a . ³⁾ Oxidation in aged boric-acid-coted vessels. P(Total) = (490-505) torr.	ES	313-753	4.7(12)	0	3200		2
71 BAK/BAL k _b .	ES	753	2.3(9)				2
(CH₃)₃C → (CH₃)₂C=CH₂ + H (a) → CH₃ + CH₃CH=CH₂ (b) → CH₂=CH₂ + CH₃CH₂ (c)							
Ethyl, 1,1-dimethyl (t-Butyl)							
81 CAN/MAR2 k _a . Azomethane-sensitized pyrolysis of Isobutane in a static system. P(Total) = (53-270) torr.	EX	584-604	4.68(14)	0	19829		1
76 BRA/WES1 ¹⁾	RL	1030-1300	7.2(3)	0	11078		1/1 1.32
76 BRA/WES2 ¹⁾	RL	1055-1325	1.27(-2)	0	-5846		1 1.41
76 BRA/WES2 ¹⁾ ¹⁾ k _b /k _c . Fit of experimental data to a proposed mechanism by computer optimization.	RL	1200	1.8				1/1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_3\text{C} + \text{O}_2 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{HO}_2$ (a) $\rightarrow (\text{CH}_3)_2\text{CO} + \text{CH}_3 + \text{O}$ (b) $\rightarrow (\text{CH}_3)_3\text{COO}$ (c)						
Ethyl, 1,1-dimethyl- (t-Butyl) + Oxygen molecule						
78 ATR/BAL k_a . Oxidation in KCl-coated vessels. P = (60-500) torr. $k_{\text{ref}}: (\text{CH}_3)_3\text{C} + \text{O}_2 \rightarrow \text{Cyclopropane oxide} + \text{OH}$	EX	470-542	1.38(1)	0	-1564	2/2
79 EVA/WAL ¹⁾ k_a/k_{ref} $k_{\text{ref}}: (\text{CH}_3)_3 + \text{H}_2 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H}$	RL	713-813	(3.5±1.0)(-1)	0	-7446±241	2/2
79 EVA/WAL ¹⁾ k_a . ¹⁾ Oxidation in KCl-coated reaction vessels.	RN	713-813	8.0(11)	0	1095±1203	2
80 WAS/BAY $(k_a + k_b)/k_{\text{ref}}$. Fast-flow reactor. Photoionization Mass-spectrometer. k measurements by Stern-Volmer plots. Channels (a) and (b) assumed to be not elementary, but to pass first through channel (c) to form the t-Butylperoxy radical which in its turn reacts with an O atom to form either Isobutene + O ₂ , or Acetone + Methyl + O ₂ . P(Isobutane) = (2.7-4.2) mtorr. P(Total) = (1.8-5.7) torr. P(O) ₀ = (4.3-8.5) mtorr. $k_{\text{ref}}: (\text{CH}_3)_3\text{C} + \text{O} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{OH}$ (c) $\rightarrow (\text{CH}_3)_2\text{CO} + \text{CH}_3$ (d)	RL	297	(2.68±0.36)(-2)			2/2
80 LEN/MCD k_c . M = He. 2-Iodo-2-methylpropane flash-photolysis. Photoionization Mass-spectrometry. P-independent for (1-4) torr. Limiting high-pressure k.	EX	298	(1.41±0.23)(13)			2
$(\text{CH}_3)_3\text{C} + \text{O}_3 \rightarrow \text{products}$ Ethyl, 1,1-dimethyl- (t-Butyl) + Ozone						
82 PAL Photoionization mass-spectrometry. $(\text{CH}_3)_3\text{C}$ generated by photodissociation of 2,4,4-Trimethylpent-1-ene. P = 2 torr.	EX	298	(3.28±0.29)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_3\text{C} + \text{H}_2 \rightarrow (\text{CH}_3)_3\text{CH} + \text{H}$						
Ethyl, 1,1-dimethyl- (t-Butyl) + Hydrogen molecule						
79 EVA/WAL Reaction in KCl-coated vessels.	DE	713-813	2.3(12)	0	8540±720	2
$(\text{CH}_3)_3\text{C} + \text{NO} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{HNO}$ (a)						
$\rightarrow (\text{CH}_3)_3\text{CNO}$ (b)						
Ethyl, 1,1-dimethyl- (t-Butyl) + Nitrogen oxide (NO)						
74 CHO/MEN k_a . Upper-limit k.	EX	600	≤3.16(10)			1
74 CHO/MEN k_b .	EX	600	(3.5±1.7)(12)			1
$(\text{CH}_3)_3\text{C} + (\text{CH}_3)_3\text{C} \rightarrow (\text{CH}_3)_2\text{CH}=\text{CH}_2 + (\text{CH}_3)_3\text{CH}$ (a)						
$\rightarrow (\text{CH}_3)_3\text{CC}(\text{CH}_3)_3$ (b)						
Ethyl, 1,1-dimethyl- (t-Butyl)						
71 FAL/SUN ¹⁾	RL	298	3.1			2/2
74 CHO/BEA ¹⁾	RL	620-690	3.0	0	0	2/2
76 PAR/QUI ¹⁾	RL	298	(2.8±0.2)			2/2
77 MCK/TUR ¹⁾	RL	483-515	(2.6±0.04)	0	0	2/2
Thermolysis in a vacuum system.						
Average ratio.						
77 MAR/MAC ¹⁾	RL	483-533	(2.9±0.2)	0	0	2/2
Thermolysis in a vacuum system.						
Average ratio.						
81 BET/LAN ¹⁾ ⁴⁾	RL	298	(2.9±0.2)			2/2 2.0
¹⁾ $k_a/k_b = k_{\text{dispr.}}/k_{\text{comb.}}$						
74 CHO/BEA ²⁾	EX	620-690	1.5(12)	0	0	2
81 BET/LAN ²⁾ ⁴⁾	EX	298	1.35(13)			2 2.0
²⁾ k_a .						
72 MCM/GOL ³⁾	EX	462	3.98(8)			2
73 HIA/BEN ³⁾	ES	373	2.51(8)			2
73 KON/MAR ³⁾	ES	773	3.98(9)			2
74 CHO/BEA ³⁾	EX	620-690	5.0(11)	0	0	2 2.0
75 PAR/QUI ³⁾	RN	298	(1.2±0.18)(12)			2
81 BET/LAN ³⁾ ⁴⁾	EX	298	4.68(12)			2 2.0
³⁾ k_b .						
81 BET/LAN ⁴⁾	EX	298	1.82(13)			2 2.0
$k_a + k_b$.						
⁴⁾ Time-resolved Infrared Spectral Photography.						
Gas-chromatography. Mass-spectrometry.						
P[(CH ₃) ₃ NO] = (15-30) torr.						
P(NO) = (3-17.5) torr.						

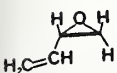
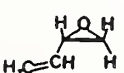
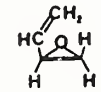
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 DEM/LDE $k_a + k_b$. Flash-photolysis. Laser-resonance-absorption. (CH ₃) ₃ C generated by flashing NH ₃ in presence of Isobutene. Data-simulation. Best-fit.	DE	298	6.5(12)			2	
CH ₃ CH ₂ CH ₂ CH ₃ → CH ₃ CH ₂ + CH ₃ CH ₂ (a) → CH ₃ CH ₂ CH ₂ + CH ₃ (b)							
Butane							
74 GOL/ALF ¹) RRKM calculation. Best fit of experimental data.	DE	1100-1250	2.51(16)	0	40715	1	
74 HUG/MAR ¹)	ES	895-981	2.0(15)	0	38852±2044	1	7.94
78 TSA4 ¹) Single-pulse shock-tube.	EX	990-1100	2.51(16)	0	41300	1	
78 TSA4 ¹) Extrapolation over the given T-range. Single-pulse shock-tube.	EX	300-1100	1.58(17)	0	43800	1	
79 PRA/ROG3 ¹) M = Ar. Butane pyrolysis in a wall-less reactor. P(Ar) = 600 torr.	EX	1025	(3.8±0.6)(-2)			1	
¹) k_a .							
74 HUG/MAR ²)	EX	895-981	2.57(15)	0	38853±1804	1	6.76
72 HAS/JOH ²) P = 0.35 torr. Butane vibrationally excited.	EX	298	(7.3±0.6)(6)			1	
72 HAS/JOH P = 1.06 torr. Butane vibrationally excited.	EX	298	(2.3±0.2)(7)			1	
80 SHE/IVA ²) Pyrolysis in a quartz reactor. Initial steps of a proposed mechanism. P = 100 torr.	EX	973-1123	1.74(14)	0	31480±1384	1	3.80
²) $k_a + k_b$.							
81 KOI/MOR2 k_b . M = Ar. Pyrolysis of Butane behind incident shock-waves. P = 20 torr.	EX	1290-1610	8.9(13)	0	36185	1	
72 ILL ³)	EX	913-1063	5.82(12)	0	28430	1	
72 ILL/SZA ³)	EX	940-1075	2.45(13)	0	30201	1	1.1
74 BAK/NOV ³) ³) k_{overall} .	EX	973-1123	1.5(12)	0	26774±805	1	
(CH ₃) ₃ CH → (CH ₃) ₂ CH + CH ₃ (a) → any other products (b)							
Propane, 2-methyl- (Isobutane)							
73 KON/MAR k_a . Estimated k.	RE	770-855	6.31(16)	0	41117	1	

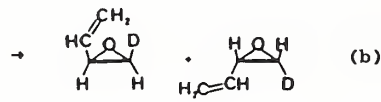
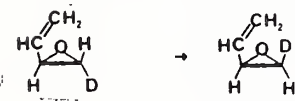
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
74 GOL/ALF k _a . RRKM calculation. Best fit of data.	DE	1100-1280	2.51(16)	0	41671	1	
80 PRA/ROG ¹)	EX	1000	(1.8±0.5)(3)			1	
80 PRA/ROG ¹) Determined on the basis of the experimental k at 1000 K and thermodynamic data.	DE	970-1031	8.4(15)	0	42985	1	
¹) k _a . M = Ar. Isobutane pyrolysis in a wall-less reactor. P(Ar) = 600 torr.							
82 KOI/MOR2 k _a . M = Ar. Pyrolysis of Isobutane behind incident shock-waves. UV-Absorption spectroscopy. P(Total) = 380 torr.	EX	1300-1800	6.31(12)	0	30599±2315	1	3.16
80 SHE/IVA k _a . Pyrolysis in a quartz reactor. Initial step of a proposed mechanism. P = 100 torr.	EX	973-1123	1.66(11)	0	24308±1158	1	3.02
72 ILL k _{overall} .	EX	913-1063	1.10(15)	0	33644	1	
78 VER/BEL k _{overall} /k _{ref} . Pyrolysis in a flow-reactor. k _{ref} : CH ₃ CH ₂ CH ₂ CH ₃ → products. Average ratio.	RL	985-1073	(9.25±0.95)(-1)			1/1	
 (CH ₃) ₃ CH [†] → (CH ₃) ₂ CH + CH ₃ Propane, 2-methyl- (Isobutane)							
71 LEX/MAR2 Discharge flow. Upper-liit ratio. (CH ₃) ₃ CH [†] formed by H + (CH ₃) ₃ C. The rate ratio given by the authors is: k/k _{ref} = (2±22)×10 ⁻¹⁰ mol.cm ⁻³ . k _{ref} : (CH ₃) ₃ CH [†] + M → (CH ₃) ₃ CH + M. P(Ar) = (4-12) torr.	RL	290	<2.46(-9)			1/2	
 CH=CCH ₂ COOH → CH ₂ =C=CH ₂ + CO ₂ 3-Butynoic acid							
76 BIG/WEA1	EX	630	1.49(-2)			1	
76 BIG/WEA1 A and B recalculated from the reported data.	EX	500-648	2.21(11)	0	19106±758	1	
 CH=CCH ₂ COOD → CHD=C=CH ₂ + CO ₂ 3-Butynoic acid-d							
76 BIG/WEA1	EX	630	5.08(-3)			1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_2\text{C}(\text{O})\text{C}(\text{O})\text{CH}_3 \rightarrow \text{CH}_2=\text{C}=\text{O} + \text{CH}_3\text{CO}$							
Butyl, 2,3-dioxo-							
75 SCH/PLA	EX	822-905	2.00(15)	0	26170	1	
 $\rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{C}=\text{O}$ (a)							
$\rightarrow \triangle + \text{CO}$ (b)							
Cyclobutanone							
72 MCG/SCH ¹⁾	EX	633-679	3.6(14)	0	26120	1	
k_a .							
72 MCG/SCH ¹⁾	EX	633-679	6.3(13)	0	28334	1	
k_b .							
¹⁾ Pyrolysis in a high-vacuum static system.							
Gas-chromatography.							
$P_0 = (1.5-38)$ torr.							
 $\rightarrow$  (a)							
$\rightarrow$  .  (b)							
(Racemic mixture)							
Oxirane, ethenyl-, (S)-							
$\rightarrow$ Furan, 2,3-tetrahydro-	(a)						
$\rightarrow$ Oxirane, ethenyl-, ($\pm$)- (racemic)	(b)						
76 CRA/LUT ¹⁾	EX	543-583	2.00(14)	0	25466 $\pm$ 604	1	7.94
k_a .							
Ring expansion.							
76 CRA/LUT ¹⁾	EX	528-548	3.39(13)	0	22245 $\pm$ 352	1	2.0
k_b .							
Racemization of the (+)-(S) form.							
$P_0 = 380$ torr.							
76 CRA/LUT ¹⁾	EX	543-583	1.26(14)	0	24056 $\pm$ 554	1	6.31
k_{overall} .							
Thermolysis at 114 torr.							
76 CRA/LUT ¹⁾	EX	580	(1.25 $\pm$ 0.01)(-4)			1	
k_{overall} .							
¹⁾ Thermolysis in a static system.							
Mass-spectrometry.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
  (Racemic mixture) 						
Oxirane-d, 3-ethenyl-, cis-, (S)-						
→ Furan-5-d, 2,3-dihydro-	(a)					
→ Oxirane-d, 3-ethenyl-, cis-, (±)-						
(racemic)	(b)					
→ Oxirane-d, 3-ethenyl-, trans-	(c)					
76 CRA/LUT ¹⁾	EX	580	1.58(-5)			1
k _a .						
Ring expansion.						
76 CRA/LUT ¹⁾	EX	580	7.24(-4)			1
k _b .						
Racemization of the (+)-(S) form.						
76 CRA/LUT ¹⁾	EX	580	1.7(-5)			1
k _c .						
Cis-trans isomerization.						
76 CRA/LUT ¹⁾	EX	580	(1.06±0.01)(-4)			1
k _{overall} .						
Thermolysis at 114 torr.						
¹⁾ Thermolysis in a static system.						
Mass-spectrometry.						
 → any other products (b)	(a)					
Oxirane-d, 3-ethenyl-, trans-						
→ Oxirane-d, 3-ethenyl-, cis-	(a)					
→ any other products	(b)					
76 CRA/LUT ¹⁾	EX	580	1.8(-5)			1
k _a .						
Trans-cis isomerization.						
76 CRA/LUT ¹⁾	EX	580	(1.07±0.01)(-4)			1
k _{overall} .						
Thermolysis at 114 torr.						
¹⁾ Thermolysis. Static system. Mass-spectrometry.						

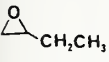
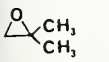
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 Oxirane, 2,2-d ₂ , 3-ethenyl- → products	EX	580	(9.8±0.1)(-5)			1	
76 CRA/LUT							
Thermolysis. Static system. Mass=spectrometry.							
P = 114 torr.							
$\text{CH}_2=\text{CHCH}_2\text{COOH} \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CO}_2$ 3-Butenoic acid	EX	634	5.0(-3)			1	
82 BIG/CLA ¹⁾							
P(Total) ₀ = 60 torr.							
82 BIG/CLA ¹⁾	EX	651	1.2(-2)			1	
P(Total) ₀ = (43-161) torr.							
¹⁾ Pyrolysis in a flow-system.							
Other k's, at various pressures, with added							
Cyclohexane, also given.							
$\text{CH}_3\text{C}(\text{O})\text{C}(\text{O})\text{CH}_3 \rightarrow \text{CH}_3\text{CO} + \text{CH}_3\text{CO}$ (a) → any other products (b)							
2,3-Butanedione							
73 KNO/SCH ¹⁾	EX	240-277	3.16(16)	0	34071±2214	1	25.1
75 SCH/PLA ¹⁾	EX	822-905	6.31(15)	0	33619±856	1	3.16
¹⁾ k _a .							
73 KNO/SCH ²⁾	EX	240-277	1.58(17)	0	33920±1158	1	5.01
75 SCH/PLA ²⁾	EX	822-905	3.98(13)	0	28083±2114	1	10.0
75 SCH/PLA ²⁾	EX	822-905	1.26(15)	0	31454±2365	1	12.59
Inhibited by Toluene.							
²⁾ k _{overall} .							
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CO} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2 + \text{CO}$ Butyl, 1-oxo-	DE	273-426	1.0(15)	0	5291±302	1	2.51
79 FOE/BER							
Butanal photolysis.							
k estimated on the basis of							
a suggested reaction scheme.							
$\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3 \rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CO}$ Butyl, 3-oxo-	RL	515-712	1.26(2)	0	8153±403	1/2	
75 KNO/SCH							
k _{ref} : $\text{CH}_2\text{CH}_2\text{COCH}_3 + \text{CH}_3\text{COCH}_2\text{CH}_2\text{COCH}_3$							
→ $\text{CH}_3\text{COCH}_2\text{CH}_3 + \text{CH}_2\text{COCH}_2\text{CH}_2\text{COCH}_3$ (a)							
→ $\text{CH}_3\text{COCH}_2\text{CH}_3 + \text{CH}_3\text{COCHCH}_2\text{COCH}_3$ (b)							

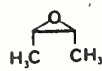
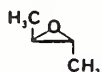
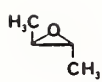
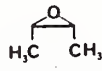
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}_2\text{CHCHO} \rightarrow \text{CH}_3 + \text{CH}_2=\text{CHCHO}$						
Propyl, 1-formyl-						
79 FOE/BER ¹⁾	RL	426	1.26(-11)			1/2
79 FOE/BER ¹⁾	RL	529	2.51(-10)			1/2
$k_{\text{ref}}:$ $\text{H}_3\text{CH}_2\text{CHCHO} + \text{CH}_3\text{CH}_2\text{CH}_2$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CHO}$						
k/k_{ref} ratios estimated on the basis of a suggested reaction scheme.						
$(\text{CH}_3)_2\text{CCHO} (+ \text{M}) \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CHO} (+ \text{M})$						
Ethyl, 1,1-dimethyl-2-oxo-						
79 BAL/CLE	RL	713	(1.4±0.2)(-2)			2/2
Oxidation in an aged boric-acid-coated vessel. P(Total) = 60 torr.						
$k_{\text{ref}}:$ $(\text{CH}_3)_2\text{CCHO} + \text{O}_2 \rightarrow (\text{CH}_3)_2\text{CO} + \text{CO} + \text{OH}$						
$\text{CH}_3\text{CH}(\text{OH})\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3 + \text{CH}(\text{OH})\text{CH}=\text{CH}_2$ (a) $\rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{H}_2\text{O}$ (b)						
3-Buten-2-ol						
73 TRE ¹⁾	EX	773-834	1.82(16)	0	34826±302	1 3.16
$k_a.$						
73 TRE ¹⁾	EX	773-834	7.94(12)	0	28032±805	1 3.16
$k_b.$						
¹⁾ Pyrolysis in a static reactor.						
$\text{CH}_3\text{OCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{HCHO} + \text{CH}_3\text{CH}=\text{CH}_2$						
1-Propene, 3-methoxy-						
77 IBU/TAK	EX	287	1.11(8)			1
$\text{CH}_3\text{CH}_2\text{OCH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CHO} + \text{CH}_2\text{CH}_2$						
Ethene, ethoxy-						
79 ROS/GOL	EX	750-1050	2.95(11)	0	21842±503	1 1.78
VLP-Pyrolysis. RRKM best-fit. High-pressure k.						
$\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_3 (+ \text{M}) \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CO} (+ \text{M})$						
2-Butanone						
75 ABU/LIS	EX	291-346	4.27(14)	0	6397±1082	1 30.9
M = $\text{CH}_3\text{CH}_2\text{CH}_3$. Limiting high-pressure k.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 $\rightarrow$ cis-CH ₃ CH=CHCH ₂ OH (a) $\rightarrow$ trans-CH ₃ CH=CHCH ₂ OH (b) $\rightarrow$ CH ₃ CH ₂ CH ₂ CHO (c) $\rightarrow$ CH ₃ CH ₂ COCH ₃ (d) $\rightarrow$ cis-CH ₃ OCH=CHCH ₃ (e) $\rightarrow$ trans-CH ₃ OCH=CHCH ₃ (f)							
Oxirane, ethyl-							
$\rightarrow$ 2-Buten-1-ol, (Z)- (a)							
$\rightarrow$ 2-Buten-1-ol, (E)- (b)							
$\rightarrow$ Butanal (c)							
$\rightarrow$ 2-Butanone (d)							
$\rightarrow$ 1-Propene, 1-methoxy, (Z)- (e)							
$\rightarrow$ 1-Propene, 1-methoxy, (E)- (f)							
75 FLO/PEN ¹⁾ k _a + k _b . Uncertainty of A is 1318.	EX	674-730	7.76(10)	0	25741±5028	1	
75 FLO/PEN ¹⁾ k _c .	EX	674-730	8.91(13)	0	28676±662	1	2.57
75 FLO/PEN ¹⁾ k _d .	EX	674-730	1.32(14)	0	29915±1263	1	6.03
75 FLO/PEN ¹⁾ k _e + k _f .	EX	674-730	1.62(12)	0	27317±1202	1	5.62
¹⁾ Thermolysis. Static system. Gas-chromatography. Mass-spectrometry. P = (5-70) torr.							
 $\rightarrow$ (CH ₃) ₂ CHCHO (a) $\rightarrow$ CH ₂ =C(CH ₃)OCH ₃ (b) $\rightarrow$ CH ₂ =C(CH ₃)CH ₂ OH (c)							
Oxirane, 2,2-dimethyl-							
$\rightarrow$ 2-Propanal, 2-methyl- (a)							
$\rightarrow$ 1-Propene, 2-methoxy- (b)							
$\rightarrow$ 2-Propen-1-ol, 2-methyl- (c)							
71 FLO/PAR1 ¹⁾ k _a .	EX	647-705	2.09(13)	0	26532±287	1	1.51
71 FLO/PAR1 ¹⁾ k _b .	EX	647-705	3.55(13)	0	28254±735	1	2.75
71 FLO/PAR1 ¹⁾ k _c .	EX	647-705	3.39(11)	0	25003±1047	1	4.68
¹⁾ Pyrolysis in a static system. Gas-chromatography.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 $\rightarrow \text{CH}_3\text{CH}(\text{OH})\text{CH}=\text{CH}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{COCH}_3$ (b) $\rightarrow (\text{CH}_3)_2\text{CHCHO}$ (c) $\rightarrow \text{CH}_3\text{CH}_2\text{OCH}=\text{CH}_2$ (d) $\rightarrow$  (e)							
Oxirane, 2,3-dimethyl- cis- (cis-2,3-Epoxybutane)							
$\rightarrow$ 3-Buten-2-ol (a)							
$\rightarrow$ 2-Butanone (b)							
$\rightarrow$ 2-Propanal, 2-methyl- Isobutyraldehyde (c)							
$\rightarrow$ Ethene, ethoxy- (Ethyl vinyl ether) (d)							
$\rightarrow$ Oxirane, 2,3-dimethyl-, trans- (trans-2,3-Epoxybutane) (e)							
71 FLO/PAR2 ¹⁾ k _a . Decyclization.	EX	668-740	1.51(12)	0	27172±1505	1	8.71
71 FLO/PAR2 ¹⁾ k _b . Decyclization.	EX	668-740	3.98(13)	0	28344±332	1	1.62
71 FLO/PAR2 ¹⁾ k _c . Decyclization.	EX	668-740	9.77(12)	0	28168±991	1	4.17
71 FLO/PAR2 ¹⁾ k _d . Decyclization.	EX	668-740	8.71(12)	0	27796±1530	1	9.12
71 FLO/PAR2 ¹⁾ k _e . Cis-trans isomerization.	EX	668-740	3.89(14)	0	31117±846	1	3.39
¹⁾ Thermolysis. Static system. Gas-chromatography. Mass-spectrometry. P ₀ = 22 torr.							
 $\rightarrow \text{CH}_3\text{CH}(\text{OH})\text{CH}=\text{CH}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_3$ (b) $\rightarrow \text{CH}_3\text{CH}_2\text{OCH}=\text{CH}_2$ (c) $\rightarrow$  (d)							
Oxirane, 2,3-dimethyl- trans- (trans-2,3-Epoxybutane)							
$\rightarrow$ 3-Buten-2-ol (a)							
$\rightarrow$ 2-Butanone (b)							
$\rightarrow$ Ethene, ethoxy- (Ethyl vinyl ether) (c)							
$\rightarrow$ Oxirane, 2,3-dimethyl-, cis- (cis-2,3-Epoxybutane) (d)							
71 FLO/PAR2 ¹⁾ k _a . Decyclization.	EX	668-740	5.37(12)	0	28007±1309	1	6.45

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
71 FLO/PAR2 ¹⁾ k _b . Decyclization.	EX	668-740	1.74(14)	0	29839±1067	1	4.47
71 FLO/PAR2 ¹⁾ k _c . Decyclization.	EX	668-740	1.70(14)	0	31595±1228	1	5.62
71 FLO/PAR2 ¹⁾ k _d . Trans-cis isomerization.	EX	668-740	4.68(14)	0	31711±8800	1	3.09
¹⁾ Thermolysis. Static system. Gas-chromatography. Mass-spectrometry. Mass-spectrometry. P ₀ = 22 torr.							
$\begin{array}{c} \text{O} \\ \\ \text{CH}_2 \\ \\ \text{CH}_3 \end{array} \rightarrow \text{HCHO} + \text{CH}_3\text{CH}=\text{CH}_2 \text{ (a)}$							
$\begin{array}{c} \text{O} \\ \\ \text{CH}_2 \\ \\ \text{CH}_3 \end{array} \rightarrow \text{CH}_3\text{CHO} + \text{CH}_2=\text{CH}_2 \text{ (b)}$							
Oxetane, 2-methyl-							
82 HAM/HOL k _a + k _b . Pyrolysis in a cylindrical Pyrex vessel with vacuum system. Gas-chromatography. P = (6.0-1.42) torr.	EX	703-756	7.76(14)	0	30047±565	1	2.29
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OH} + \text{CH}_2=\text{CH}_2$							
Acetic acid ethyl ester (Ethyl acetate)							
72 BEA/GOL2 VLPP of Ethyl acetate in Ar, in a triple aperture quartz reactor. Gas-chromatography. Mass-spectrometry. The data agree well with the high-P Arrhenius expression determined by Blades and Gilderson, Can. J. Chem. 38, 1407 (1960).	EX	772-1156	3.98(12)	0	24157	1	
75 TAY Pyrolysis. Acetic acid decomposes further into CO ₂ + CH ₄ in a fast reaction.	EX	650-700	3.16(12)	0	24056±503	1	2.0
76 DEB/TAY	EX	650-700	3.16(12)	0	24006	1	
82 KEL/FET Thermolysis in a flow-reactor. P = 750 torr.	EX	940-1050	3.92(12)	0	24538	1	
82 MCM/LEW ¹⁾ k determined versus Isobutyl bromide.	RN	950-1000	5.0(12)	0	24912	1	
82 MCM/LEW ¹⁾ k determined versus Isopropyl acetate.	RN	950-1000	6.31(12)	0	24660	1	
¹⁾ Laser-powered homogeneous pyrolysis of an Ethyl acetate/Isopropyl acetate/Isobutyl bromide/SF ₆ /CO ₂ mixture. Gas-chromatography. P(Acetate, or Bromide) ~ 1.0 torr. P(SF ₆) = 4 torr. P(CO ₂) = 93 torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref)), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{OC}(\text{O})\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{OH} + \text{CO}_2 + \text{CH}_2=\text{CH}_2$ Carbonic acid ethyl methyl ester							
76 CRO/HUN	EX	581-667	5.25(11)	0	21892	1	
$\text{CH}_3\text{CH}(\text{OH})\text{CHCH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{CH}(\text{OH})\text{CH}(\text{O}_2)\text{CH}_3$ Propyl, 2-hydroxy-1-methyl- + Oxygen molecule							
80 LEN/MCD M = He. 3-Iodo-2-butanol flash-photolysis. Photoionization Mass-spectrometer. Limiting high-pressure k. P-independent for (1-4) torr.	EX	298	(1.69±1.08)(13)			2	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{O} \rightarrow \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$ Butoxy							
80 ROS Butyl nitrite/ NO_2 photolysis at 366 nm. $k_{\text{ref}}: \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{O} + \text{NO}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{ONO}_2$	RL	298	(2.8±0.5)(-8)			1/2	
81 COX/FAT HONO/ N_2/O_2 /Butane photolysis. P = 760 torr. $k_{\text{ref}}: \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{O} + \text{O}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CHO} + \text{HO}_2$	RL	296	(2.49±0.83)(-5)			1/2	
$\text{CH}_3\text{CH}_2\text{CH}(\text{O}\cdot)\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CHO}$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CHO} + \text{CH}_3$ (b) Propoxy, 1-methyl-							
75 BAT/MCC ¹⁾	ES	393-473	1.0(16)	0	8807	1	
76 BAT/MCC2 ¹⁾	ES	403-433	6.31(14)	0	7700	1	
79 BAT ¹⁾ Static system.	ES	403-433	7.94(14)	0	7700±503	1	3.16
81 COX/FAT ¹⁾ HONO/ N_2/O_2 /Butane photolysis. P = 760 torr. $k_{\text{ref}}: \text{CH}_3\text{CH}_2\text{CH}(\text{O}\cdot)\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_3 + \text{HO}_2$ ¹⁾ k_a .	RL	296	(4.32±0.58)(-6)			1/2	
79 BAT k_b . Static system.	ES	403-433	7.9(14)	0	9562	1	
$\text{CH}_3\text{CH}_2\text{CH}(\text{O}\cdot)\text{CH}_3 + \text{NO} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_3 + \text{HNO}$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{ONO}$ (b) Propoxy, 1-methyl- + Nitrogen oxide (NO)							
75 BAT/MCC ¹⁾	ES	393-473	3.98(12)	0	0±503	2	3.16
76 BAT/MCC2 ¹⁾ ¹⁾ k_a .	ES	403-433	6.31(12)	0	0±503	2	2.51
76 BAT/MCC2 k_b . Same data given in 75 BAT/MCC.	ES	403-433	2.51(13)	0	0±503	2	2.51

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}_2\text{CH}(\text{O}\cdot)\text{CH}_3 + \text{NO}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_3 + \text{HONO}$ (a)						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{ONO}_2$ (b)						
Propoxy, 1-methyl- + Nitrogen oxide (NO_2)						
80 ROS	RL	298	(8.0±8.0)(-2)			2/2
k_a/k_b . sec-Butyl nitrite/ NO_2 photolysis at 366 nm. Gas-chromatography.						
$(\text{CH}_3)_3\text{CO} \rightarrow (\text{CH}_3)_2\text{CO} + \text{CH}_3$						
Ethoxy, 1,1-dimethyl- (t-Butoxy)						
71 CAD/TRO	EX	373-423	2.34(13)	0	8444±746	1 6.61
Limiting high-pressure k.						
75 BAT/MCC	ES	393-473	3.98(15)	0	8606	1
76 BAT/MIL	ES	393-433	4.0(15)	0	8556	1
79 BAT	ES	393-433	3.16(15)	0	8556±503	1 3.16
Static system.						
81 CHO/BEN	RE	248-450	1.26(14)	0	7700	1
Recommended by the authors.						
Critical evaluation.						
81 KIR/PAR ¹⁾	RL	298	5.0(14)			1/2
81 KIR/PAR ¹⁾	RL	333	1.0(16)			1/2
¹⁾ Azo-t-butane/ O_2 photolysis. Gas-chromatography. Approximate rate ratios. k_{ref} : $(\text{CH}_3)_3\text{CO} + (\text{CH}_3)_3\text{COOH} \rightarrow (\text{CH}_3)_3\text{COH} + (\text{CH}_3)_3\text{CO}_2$						
82 BAT/ROB ²⁾	EX	403-443	3.98(14)	0	8002±604	1 3.98
82 BAT/ROB ²⁾	CO	403-443	7.94(14)	0	8354	1
RRKM best-fit.						
²⁾ M = CF_4 , SF_6 , N_2 , Ar. Limiting high-pressure k. Static system. $(\text{CH}_3)_3\text{C}$ decomposition in presence of NO and an inert gas. $(\text{CH}_3)_3\text{C}$ generated by decomposition of di-t-Butyl peroxide. P[inert gas] = (25-1500) torr.						
$(\text{CH}_3)_3\text{CO} + \text{NO} \rightarrow (\text{CH}_3)_3\text{CONO}$						
Ethoxy, 1,1-dimethyl- (t-Butoxy) + Nitrogen oxide (NO)						
74 BAT/MIL	ES	393-473	2.51(13)	0	0±503	2 2.51
75 BAT/MCC	ES	393-473	2.51(13)	0	0±503	2 2.51
75 MEN/GOL	DE	300	6.31(12)	0	0	2
B ~ 0 assumed. Estimated k.						
77 BAR/BEN2	ES	650-800	6.31(12)			2
VLP-Pyrolysis. RRKM best-fit estimate.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_3\text{CO} + \text{HCHO} \rightarrow (\text{CH}_3)_3\text{COH} + \text{CHO}$						
Ethoxy, 1,1-dimethyl- (t-Butoxy) + Formaldehyde						
81 ALA/SEL ¹⁾ Calculated by using: $\log A_{\text{ref}} = 17.5(\text{c}^3\text{mol}^{-1}\text{s}^{-1})$.	RN	399-434	7.94(12)	0	2322±277	2 1.58
81 ALA/SEL ¹⁾ Calculated by using: $\log A_{\text{ref}} = 18.5(\text{c}^3\text{mol}^{-1}\text{s}^{-1})$.	RN	399-434	1.58(13)	0	1985±265	2 1.58
¹⁾ Cylindrical Pyrex vessel. Static system. ($\text{CH}_3)_3\text{CO}$ generated by thermolysis of Di-t-butyl peroxide. Mass-spectrometry. P(Total) = (20-200) torr. $k_{\text{ref}}: (\text{CH}_3)_3\text{O} + \text{M} \rightarrow \text{CH}_3 + (\text{CH}_3)_2\text{CO} + \text{M}$.						
$(\text{CH}_3)_3\text{CO} + \text{CH}_3\text{CHO} \rightarrow (\text{CH}_3)_3\text{COH} + \text{CH}_2\text{CHO}$ (a) $\rightarrow (\text{CH}_3)_3\text{COH} + \text{CH}_3\text{CO}$ (b)						
Ethoxy, 1,1-dimethyl- (t-Butoxy) + Acetaldehyde						
81 ALA/SEL ¹⁾ $k_a + k_b$. Sum of rate constants determined relative to the reaction: $(\text{CH}_3)_3\text{CO} + \text{M} \rightarrow \text{CH}_3 + (\text{CH}_3)_2\text{CO} + \text{M}$	RN	399	(1.1±0.1)(10)			2
81 ALA/SEL ¹⁾ $k_a + k_b$. Sum of rate constants determined relative to the reaction: $(\text{CH}_3)_3\text{CO} + \text{M} \rightarrow \text{CH}_3 + (\text{CH}_3)_2\text{CO} + \text{M}$	RN	434	(1.6±0.1)(10)			2
81 ALA/SEL ¹⁾ k_a/k_b . Estimated ratio.	RL	399	(4.7±0.8)(-2)			2/2
81 ALA/SEL ¹⁾ k_a .	ES	399	(4.9±1.5)(8)			2
81 ALA/SEL ¹⁾ k_a .	ES	434	(7.2±0.2)(8)			2
81 ALA/SEL ¹⁾ k_b .	ES	399	(1.0±0.7)(10)			2
81 ALA/SEL ¹⁾ k_b .	ES	434	(1.5±0.6)(10)			2
¹⁾ Cylindrical Pyrex vessel. Static system. ($\text{CH}_3)_3\text{CO}$ generated by thermolysis of Di-t-butyl peroxide. Mass-spectrometry.						
$(\text{CH}_3)_3\text{CO} + \text{CD}_3\text{CHO} \rightarrow (\text{CH}_3)_3\text{COD} + \text{CD}_2\text{CHO}$ (a) $\rightarrow (\text{CH}_3)_3\text{COH} + \text{CD}_3\text{CO}$ (b)						
Ethoxy, 1,1-dimethyl- (t-Butoxy) + Acetaldehyde-2,2,2-d ₃						
81 ALA/SEL ¹⁾ k_a/k_b .	RL	399	(1.0±0.2)(-2)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 ALA/SEL ¹⁾ k _a . Estimated k. ¹⁾ Pyrex vessel with vacuum system. (CH ₃) ₃ CO generated by thermolysis of Di-t-butyl peroxide. Mass-spectrometry.	RN	399	(1.1±0.3)(8)			2
(CH ₃) ₃ CO + (CH ₃) ₂ CO → (CH ₃) ₃ COH + CH ₂ C(O)CH ₃ Ethoxy, 1,1-dimethyl- (t-Butoxy) + 2-Propanone						
81 ALA/SEL ¹⁾ Calculated by using: logA _{ref} = 17.5(c ³ mol ⁻¹ s ⁻¹).	RN	399-434	1.26(13)	0	3091±156	2 1.26
81 ALA/SEL ¹⁾ Calculated by using: logA _{ref} = 18.5(c ³ mol ⁻¹ s ⁻¹).	RN	399-434	3.16(13)	0	2874±397	2 2.0
¹⁾ Di-tert-butyl peroxide thermolysis in a Pyrex vessel with vacuum system. Mass-spectrometry. k _{ref} : (CH ₃) ₃ CO + M → CH ₃ + (CH ₃) ₂ CO + M.						
(CH ₃) ₃ CO + (CD ₃) ₂ CO → (CH ₃) ₃ COD + CD ₂ C(O)CD ₃ Ethoxy, 1,1-dimethyl- (t-Butoxy) + 2-Propanone-1,1,1,3,3,3-d ₆						
81 ALA/SEL ¹⁾ Calculated by using: logA _{ref} = 17.5(c ³ mol ⁻¹ s ⁻¹).	RN	399-434	1.58(13)	0	3801±361	2 1.58
81 ALA/SEL ¹⁾ Calculated by using: logA _{ref} = 18.5(c ³ mol ⁻¹ s ⁻¹).	RN	399-434	2.00(13)	0	3271±337	2 2.0
¹⁾ Di-tert-butyl peroxide thermolysis in a Pyrex vessel with vacuum system. Mass-spectrometry. k _{ref} : (CH ₃) ₃ O + M → CH ₃ + (CH ₃) ₂ CO + M.						
(CH ₃) ₃ CO + (CH ₃) ₃ CH → (CH ₃) ₃ COH + (CH ₃) ₃ C Ethoxy, 1,1-dimethyl- (t-Butoxy) + Propane, 2-methyl- (Isobutane)						
82 PAR/SON Reaction in a static-photolysis reactor. (CH ₃) ₃ CO generated by UV-photolysis of Di-t-butyl peroxide. k determined relative to the reaction: (CH ₃) ₃ CO → CH ₃ + (CH ₃) ₂ CO	RN	316-338	2.51(11)	0	2164	2 3.16
(CH ₃) ₃ CO ₂ + NO → products Ethyldioxy, 1,1-dimethyl- + Nitrogen oxide (NO)						
78 ANA/SMI2 Azoisobutane/O ₂ /NO ₂ flash-photolysis. [Azoisobutane] = (1.0-3.0)×10 ¹⁷ molec.cm ⁻³ . [NO] = (0.1-1.0)×10 ¹⁶ molec.cm ⁻³ . Lower-limit k.	EX	298	>6.02(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A'(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_3\text{CO}_2 + \text{NO}_2 \rightarrow \text{products}$						
Ethylidioxy, 1,1-dimethyl- + Nitrogen oxide (NO_2)						
78 ANA/SMI2 Azoisobutane/ O_2/NO_2 flash-photolysis. [Azoisobutane] = $(1-3) \times 10^{17}$ molec. cm^{-3} . Lower-limit k.	EX	298	>3.01(11)			2
$(\text{CH}_3)_3\text{CO}_2 + (\text{CH}_3)_3\text{CO}_2 \rightarrow (\text{CH}_3)_3\text{CO} + (\text{CH}_3)_3\text{CO} + \text{O}_2$ (a) $\rightarrow (\text{CH}_3)_3\text{COOC}(\text{CH}_3)_3 + \text{O}_2$ (b)						
Ethylidioxy, 1,1-dimethyl-						
75 PAR k_a . Unreported T assumed to be 298 K.	EX	298	(2.17 $\pm$ 0.48)(6)			2
81 KIR/PAR ¹⁾	RL	298	1.4(-1)			2/2
81 KIR/PAR ¹⁾	RL	333	5.0(-2)			2/2
¹⁾ k_b/k_a . Azo-t-butane/ O_2 photolysis. Approximate rate ratios. Gas-chromatography.						
78 ANA/SMI2 k_{overall} . Azoisobutane/ O_2 flash-photolysis. [Azoisobutane] = $(1-3) \times 10^{17}$ molec. cm^3 .	EX	298	(1.57 $\pm$ 0.47)(7)			2
$(\text{CH}_3)_2\text{CCH}_2\text{OOH} \rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{OH} + \text{OH}$ (a) $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CHO} + \text{OH} + \text{H}_2$ (b) $\rightarrow (\text{CH}_3)_2\text{CHCHO} + \text{OH}$ (c) $\rightarrow \begin{array}{c} \text{O} \\ \diagup \quad \diagdown \\ \text{CH}_2 \quad \text{CH}_2 \end{array} + \text{OH}$ (d)						
Ethyl, 1-(hydroperoxymethyl)-1-methyl-						
$\rightarrow$ 2-Propen-1-ol, 2-methyl- + Hydroxyl (a)						
$\rightarrow$ 2-Propenal, 2-methyl- (Methacrolein) + Hydroxyl + Hydrogen molecule (b)						
$\rightarrow$ Propanal, 2-methyl- + Hydroxyl (c)						
$\rightarrow$ Oxirane, 2,2-dimethyl- + Hydroxyl (d)						
78 BAK/BAL ¹⁾ k_a .	ES	753	1.3(5)			1 2.0
78 BAK/BAL ¹⁾ k_b .	ES	753	1.3(5)			1 2.0
78 BAK/BAL ¹⁾ k_c .	ES	753	4.2(5)			1 2.0
78 BAK/BAL ¹⁾ k_d .	ES	753	1.8(6)			1 2.0
¹⁾ Aged boric-acid-coated vessels. P(Total) = (490-505) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$(\text{CH}_3)_2\text{CHCH}_2\text{O}_2 \rightarrow (\text{CH}_3)_2\text{CCH}_2\text{OOH} \quad (\text{a})$ $\rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{OOH})\text{CH}_3 \quad (\text{b})$							
Propyldioxy, 2-methyl-							
78 BAK/BAL ¹⁾ k _a /k _b .	RL	753	(4.08±0.41)			1/1	
78 BAK/BAL ¹⁾ k _a .	RN	753	1.8(5)			1	
78 BAK/BAL ¹⁾ k _b .	RN	753	4.5(4)			1	
¹⁾ Aged boric-acid-coated vessels. Rate constants computed by Benson's group additivity method. P(Total) = (490-505) torr.							
$(\text{CH}_3)_2\text{C}(\text{OO}\cdot)\text{CH}_2\text{OOH} \rightarrow (\text{CH}_3)_2\text{CO} + \text{HCHO} + \text{HO}_2$							
Ethylidioxy, 1-(hydroperoxymethyl)-1-methyl-							
76 BAK/BAL Aged boric-acid-coated vessels. P(Total) = (490-505) torr.	ES	753	2.5(6)			1	2.0
$(\text{CH}_3)_3\text{COH} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H}_2\text{O} \quad (\text{a})$ $\rightarrow \text{CH}_3 + (\text{CH}_3)_2\text{C(OH)} \quad (\text{b})$							
2-Propanol, 2-methyl- (t-Butanol)							
71 GON/LEW ¹⁾	EX	753-833	2.50(5)	0	15136	1	
71 DOR/MCG ¹⁾ Pyrolysis. M = He + Ar. Reflected shock-waves.	EX	935-1397	2.24(13)	0	30448±50	1	1.58
74 LEW/KEI ¹⁾ Pyrolysis. M = He + Ar. Reflected shock-waves. P = (370-1560) torr.	EX	920-1175	3.98(14)	0	33317±503	1	1.58
¹⁾ k _a .							
76 TSA1 k _b .	ES	1080-1165	6.31(16)	0	40900	1	
$(\text{CH}_3\text{CH}_2)_2\text{O} \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2\text{O}$							
Ethane, 1,1'-oxybis- (Diethyl ether)							
77 SER/LAB Thermolysis.	ES	763-823	5.0(15)	0	40765	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{SCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{HCHS} + \text{CH}_3\text{CH}=\text{CH}_2$						
1-Propene, 3-(methylthio)- $\rightarrow$ Methanethial + 1-Propene						
82 MAR/ROP2 Pyrolysis in a stirred-flow system. Gas-chromatography. Mass-spectrometry. P = (2-15) torr. HCHS polymerizes, to give probably the cyclic trimer 1,3,5-Trithiane.	EX	588-691	1.70(11)	0	19426 $\pm$ 361	1 1.78
$\text{CH}_3\text{C}(\text{S})\text{SCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CS}_2 + \text{CH}_2=\text{CH}_2$						
Ethane(dithioic) acid ethyl ester						
78 ALA/BIG ¹⁾	EX	629	1.80(-3)			1
78 ALA/BIG ¹⁾ A and B recalculated from the reported data.	EX	651-716	8.83(12)	0	22725	1
¹⁾ Pyrolysis in a flow-reactor. Gas-chromatography. IR-, and NMR-spectrometry.						
$\text{CH}_3\text{C}(\text{O})\text{SCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{COS} + \text{CH}_2=\text{CH}_2$						
Ethanethioic acid S-ethyl ester						
72 OEL/TIN Elimination by thermolysis.	EX	763-841	2.51(12)	0	25365	1
$\text{CH}_3\text{C}(\text{S})\text{OCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{COS} + \text{CH}_2=\text{CH}_2$ (a) $\rightarrow \text{CH}_3\text{C}(\text{O})\text{SCH}_2\text{CH}_3$ (b)						
Ethanethioic acid O-ethyl ester						
72 OEL/TIN k_a . Elimination by thermolysis. Channel (a) is predominant. T-range assumed to be the same as that of Ethanedithioic acid S-ethyl ester (see above).	EX	763-841	3.16(12)	0	20735	1
75 BIG/GAB ¹⁾ k_a . Elimination.	EX	629	1.15(-2)			1
75 BIG/GAB ¹⁾ k_b . Isomerization.	EX	629	1.73(-3)			1
75 BIG/GAB ¹⁾ $k_a + k_b$. Overall reaction.	EX	635	1.78(-2)			1
75 BIG/GAB ¹⁾ $k_a + k_b$. Overall reaction.	EX	625-653	3.55(12)	0	20886	1
¹⁾ Flow reactor pyrolysis.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{OC}(\text{S})\text{OCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{OH} + \text{COS} + \text{CH}_2=\text{CH}_2$						
Carbonothioic acid O-ethyl O-methyl ester						
82 ALA/BIG ¹⁾	EX	629	1.3(-2)			1
82 ALA/BIG ¹⁾	EX	570-660	3.22(10)	0	17950	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a flow reactor.						
IR-spectrometry.						
P = (2-800) torr.						
$\text{CH}_3\text{OC}(\text{O})\text{SCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{OH} + \text{COS} + \text{CH}_2=\text{CH}_2$						
Carbonothioic acid S-ethyl O-methyl ester						
79 ALA/BIG ¹⁾	EX	629	7.75(-7)			1
79 ALA/BIG ¹⁾	EX	763-823	1.24(13)	0	27813±722	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a flow-reactor.						
Flow-tube method.						
IR-spectrometry.						
$\text{CH}_3\text{CH}_2\text{OC}(\text{O})\text{SCH}_3 \rightarrow \text{CH}_2=\text{CH}_2 + \text{CO}_2 + \text{CH}_3\text{SH}$						
Carbonothioic acid O-ethyl S-methyl ester						
79 ALA/BIG ¹⁾	EX	7629	1.0(-4)			1
79 ALA/BIG ¹⁾	EX	763-823	1.64(12)	0	23483±721	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a flow-reactor.						
Flow-tube method.						
IR-spectrometry.						
$\text{CH}_3\text{SC}(\text{S})\text{OCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{SH} + \text{COS} + \text{CH}_2=\text{CH}_2$						
Carbonodithioic acid O-ethyl S-methyl ester						
82 ALA/BIG ¹⁾	EX	629	1.4(-2)			1
82 ALA/BIG ¹⁾	EX	590-620	8.95(11)	0	19995	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a flow reactor.						
IR-spectrometry.						
P = (2-800) torr.						
$\text{CH}_2=\text{CHCH}_2\text{NC} \rightarrow \text{CH}_2=\text{CHCH}_2\text{CN}$						
1-Propene, 3-isocyano-						
79 GLI/PRI	EX	403-493	5.89(14)	0	20533±302	1 2.0
Thermal isomerization in a Pyrex bulb.						
Gas-chromatography.						
P = 20 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
cis-CH₃CH=CHCN → trans-CH₃CH=CHCN							
2-Butenenitrile, (Z)- (cis-Crotononitrile)							
→ 2-Butenenitrile, (E)-							
75 MAR/JEF	EX	1060-1380	1.58(13)	0	29190±1007	1	2.0
M = Ar. Single-pulse shock-tube isomerization.							
Limiting high-pressure k.							
P(Ar) = (200-340) torr.							
 → cis-CH ₃ CH=CHCN (a)							
→ trans-CH ₃ CH=CHCN (b)							
→ CH ₂ =CHCH ₂ CN (c)							
Cyclopropanecarbonitrile (Cyclopropyl cyanide)							
→ 2-Butenenitrile, (Z)- (cis-Crotononitrile) (a)							
→ 2-Butenenitrile, (E)- (trans-Crotononitrile) (b)							
→ 3-Butenenitrile (Allyl cyanide) (c)							
73 LUC/ROB ¹⁾	EX	660-760	1.02(14)	0	28580±168	1	1.29
k _a .							
73 LUC/ROB ¹⁾	EX	660-760	1.23(14)	0	29313±108	1	1.17
k _b .							
73 LUC/ROB ¹⁾	EX	660-760	3.89(14)	0	30372±217	1	1.35
k _c .							
73 LUC/ROB ¹⁾	EX	660-760	3.80(14)	0	29109±144	1	1.20
k _a + k _b + k _c .							
¹⁾ Thermal isomerization in a silica reaction vessel with Pyrex vacuum system.							
Gas-chromatography.							
CH₃CH₂CH₂CN → CH₃CH₂ + CH₂CN							
Butanenitrile							
75 KIN/GOD2	EX	1090-2050	2.51(15)	0	38601±856	1	2.0
(CH₃)₂CHCN → CH₃CH=CH₂ + HCN (a)							
→ CH₃CHCN + CH₃ (b)							
Propanenitrile, 2-methyl-							
73 DAS/EMO	EX	820-928	1.58(12)	0	32280±523	1	1.12
k _a .							
75 KIN/GOD1	EX	1074-1253	7.94(13)	0	38349±1007	1	2.0
k _a .							
75 KIN/GOD1	EX	1074-1250	5.01(15)	0	39758±1007	1	2.0
k _b .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_2=\text{CHCH}_2\text{NHCH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_2=\text{NH}$ 2-Propen-1-amine, N-methyl- (N-Allyl-N-methylamine)- → 1-Propene + Methanimine							
74 VIT/EGG2 Pyrolysis in a static system. Gas-chromatography. $P(\text{CH}_2=\text{CHCH}_2\text{NHCH}_3) = (9-71) \text{ torr.}$	EX	602-694	2.34(11)	0	21832±815	1	3.63
$\text{CH}_3\text{N}=\text{NCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3 + \text{CH}_2\text{CH}=\text{CH}_2 + \text{N}_2$ Diazene, methyl-(2-propenyl)-							
72 CRA/TAK ¹⁾ $k_{\text{ref}}: \text{CH}_3\text{N}=\text{NCD}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3 + \text{CD}_2\text{CH}=\text{CH}_2 + \text{N}_2$	RL	399	(1.28±0.05)			1/1	
72 CRA/TAK ¹⁾ Uninhibited k.	EX	436-456	3.24(14)	0	17816±352	1	2.09
72 CRA/TAK ¹⁾ In presence of ¹⁵ NO.	EX	383-403	2.29(14)	0	17866±352	1	2.40
¹⁾ Thermolysis. Mass-spectrometry. Gas-chromatography. $P(\text{Total}) = (50-60) \text{ torr.}$							
$\text{CH}_3\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2 + \text{N}_2$ Diazene, diethyl- (Azoethane)							
73 PER/BEA RRKM fit of experimental data.	EX	700-950	2.51(16)	0	25013±503	1	
77 MAR/MAC ¹⁾	EX	553-673	1.58(14)	0	22373±241	1	1.58
80 ACS/PET ¹⁾	EX	523-623	6.31(15)	0	24670±180	1	1.26
¹⁾ Azoethane thermolysis in a vacuum system.							
$\text{CH}_3\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_3^* \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2 + \text{N}_2$ Diazene, diethyl- (Azoethane)							
77 CHE/ORE High-pressure photolysis of Azoethane in He. RRKM data fit on the basis of a proposed mechanism. Azoethane is assumed to be in a vibrationally excited T ₁ electronic state. Lower-limit k. $P(\text{He}) = (0-150) \text{ atm.}$ $P(\text{CO}_2) = (0-45) \text{ atm.}$	EX	298	6.0(9)			1	
$(\text{CH}_3)_2\text{NN}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{N} + (\text{CH}_3)_2\text{N}$ Hydrazine, tetramethyl-							
72 GOL/SOL RRKM fit of experimental data.	EX	720-930	2.51(17)	0	27177	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{NCC(O)OCH}_2\text{CH}_3 \rightarrow \text{HCN} + \text{CO}_2 + \text{CH}_2=\text{CH}_2$							
Carbonocyanidic acid ethyl ester (Ethyl cyanoformate)							
74 BAR/DES Thermolysis.	EX	613-678	2.75(11)	0	21439±307	1	1.78
$(\text{CH}_3)_3\text{CNO} \rightarrow (\text{CH}_3)_3\text{C} + \text{NO}$							
Propane, 2-methyl-2-nitroso-							
74 CHO/MEN	EX	550-850	3.98(15)	0	18118±503	1	3.2
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{ONO} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{O} + \text{NO}$							
Nitrous acid butyl ester (n-Butyl nitrite)							
78 BAL/GOL VLP-Pyrolysis. Best RRKM data-fit.	EX	590-750	3.16(16)	0	20634	1	
$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{ONO} \rightarrow \text{CH}_3\text{CH}_2\text{COCH}_3 + \text{HONO} \quad (\text{a})$							
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{O}^\cdot)\text{CH}_3 + \text{NO} \quad (\text{b})$							
Nitrous acid 1-methylpropyl ester (s-Butyl nitrite)							
76 BAT/MCC2 k_a .	EX	403-433	6.31(12)	0	18017±403	1	3.16
75 BAT/MCC k_b .	EX	393-473	1.26(16)	0	20735±403	1	2.51
76 BAT/MCC2 k_b .	EX	403-433	1.58(16)	0	20584±403	1	2.51
76 BAT/MCC2 $k_a + k_b$.	EX	403-433	5.01(15)	0	19926±403	1	3.16
$(\text{CH}_3)_3\text{CONO} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{HONO} \quad (\text{a})$							
$\rightarrow (\text{CH}_3)_3\text{CO} + \text{NO} \quad (\text{b})$							
Nitrous acid 1,1-dimethylethyl ester (t-Butyl nitrite)							
76 BAT/MIL k_a . Same data given in 74 BAT/MIL and 75 BAT/MCC.	EX	393-433	7.9(12)	0	16910±403	1	2.51
75 MEN/GOL k_b . RRKM fit of experimental data.	CO	300	6.31(15)	0	19779	1	
76 BAT/MIL k_b . Same data given in 74 BAT/MIL and 75 BAT/MCC.	EX	393-433	2.0(16)	0	20282±403	1	2.51

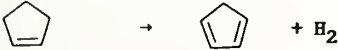
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 BAR/BEN2 k _b . VLF-Pyrolysis. RRKM best-fit estimate.	ES	650-800	6.31(15)	0	19779	1	
76 BAT/MIL k _a + k _b . Same data given in 74 BAT/MIL and 75BAT/MCC.	EX	393-433	5.0(14)	0	18218±403	1	2.51
 (CH ₃) ₃ CONO ₂ → (CH ₃) ₃ CO + NO ₂ Nitric acid 1,1-dimethylethyl ester (t-Butyl nitrate)							
76 BAT/MIL	ES	393-433	7.9(15)	0	20232	1	
 (CH ₃ CH ₂) ₂ NO + NO ₂ → CH ₃ CH ₂ N(1O)=CHCH ₃ + HONO Nitroxide, diethyl- + Nitrogen oxide (NO ₂)							
82 GLE/HEI Oxidation of Diethylhydroxylamine by NO ₂ in a variable path-length IR gas-cell. IR-Spectrometry. [(CH ₃ CH ₂) ₂ NOH] = (25-45) mtorr. [CH ₃ CHO] = (0-32) mtorr. [NO ₂] = (15-236) mtorr. [HONO] = (11-15) mtorr.	ES	298	≈1.51(6)			2	
 (CH ₃ CH ₂) ₂ NOH + NO ₂ → (CH ₃ CH ₂) ₂ NO + HONO (a) Ethanamine, N-ethyl-N-hydroxy- + Nitrogen oxide (NO ₂)							
82 GLE/HEI k _a . Oxidation of Diethylhydroxylamine by NO ₂ in a variable path-length IR gas-cell. IR-Spectrometry. [(CH ₃ CH ₂) ₂ NOH] = (25-45) mtorr. [CH ₃ CHO] = (0-32) mtorr. [NO ₂] = (15-236) mtorr. [HONO] = (11-15) mtorr.	ES	298	(3.31±0.60)(6)			2	
74 JAY/SIM k _{overall} . Dark reaction of (CH ₃ CH ₂) ₂ NOH (diluted in CO ₂) with NO ₂ (diluted in O ₂), in a cylindrical vessel with conventional high-vacuum system. P(Diethylhydroxylamine) = 2.2 mtorr. P(NO ₂) = 19.3 mtorr.	EX	298	2.71(6)			2	
 (CH ₃ CH ₂ NO) ₂ → CH ₃ CH ₂ NO + CH ₃ CH ₂ NO Diazene, diethyl-, 1,2-dioxide- (Nitrosoethane dimer)							
72 TAN/LAM	RN	314	(4.1±0.6)(03(			1	

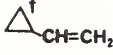
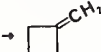
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}\equiv\text{CH} \rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{C}=\text{CH}_2$							
1-Pentyne							
81 KIN1 1-Pentyne thermolysis. VLP-Pyrolysis system. Mass-spectrometry.	EX	923-1154	6.31(12)	0	28686±1007	1	2.51
$\text{CH}_3\text{CH}_2\text{C}\equiv\text{CCH}_3 \rightarrow \text{CH}_3 + \text{CH}_2\text{C}\equiv\text{CCH}_3$							
2-Pentyne							
82 NGU/KIN1 2-Pentyne thermolysis. VLP-Pyrolysis system. Mass-spectrometry. High-pressure k. 1) Curved Arrhenius plot. For 1100 K the authors give: $k = 1.0 \times 10^{16} \exp(-36537 \pm 1007) \text{ s}^{-1}$.	EX	988-1234	1)	1)	1)	1	
$(\text{CH}_3)_2\text{CHC}\equiv\text{CH} \rightarrow \text{CH}_3\text{CHC}\equiv\text{CH} + \text{CH}_3$ (a) $\rightarrow (\text{CH}_3)_2\text{C}=\text{C}=\text{CH}_2$ (b)							
1-Butyne, 3-methyl-							
81 NGU/KIN 1) k_a . Thermolysis.	EX	940-1222	2.00(16)	0	36034±503	1	2.0
81 NGU/KIN 1) k_b . Thermal isomerization.	EX	940-1222	1.58(13)	0	30448±503	1	3.98
1) Thermolysis of 3-Methyl-1-butyne in a VLP-Pyrolysis system. Mass-spectrometry.							
$\text{cis-CH}_3\text{CH}=\text{CHCH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHCH}=\text{C}=\text{CH}_2 + \text{H}_2$ (a) $\rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}=\text{CH}_2$ (b)							
1,3-Pentadiene, (Z)-							
82 NGU/KIN2 k_a . cis-1,3-Pentadiene unimolecular thermolysis. VLP-Pyrolysis system. Mass-spectrometry. 1) Curved Arrhenius plot. For 1100 K the authors give: $k = 1.0 \times 10^{13} \exp(-32461 \pm 1007) \text{ s}^{-1}$.	EX	1002-1235	1)	1)	1)	1	
71 FRE/LAM k_b . Thermal isomerization in a static system. Gas-chromatography. k is P-independent between 0.75 and 75 torr. Determined from the Equi- librium constant and the sum of k_b and k_{-b} .	DE	473-517	3.09(13)	0	26210±301	1	1.55
75 MAR/JEF k_b . M = Ar. Single-pulse shock-tube Isomeri- zation. Limiting high-pressure k. P(Ar) = (200-340) torr.	EX	1060-1280	3.98(13)	0	26673±1007	1	2.0

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{cis-CH}_2=\text{CHCH}=\text{CHCH}_3^\dagger \rightarrow \text{trans-CH}_2=\text{CHCH}=\text{CHCH}_3^\dagger$							
1,3-Pentadiene, (Z)-							
75 CRA/ROS	RL	298	(1.3±0.1)			1/1	
$\text{cis-CH}_2=\text{CHCH}=\text{CHCH}_3^\dagger$ formed by:							
$^1\text{CH}_2 + \text{CH}_2=\text{CHCH}=\text{CH}_2$							
$k_{\text{ref}}:$							
$\text{trans-CH}_2=\text{CHCH}=\text{CHCH}_3^\dagger \rightarrow \text{cis-CH}_2=\text{CHCH}=\text{CHCH}_3^\dagger$							
$\text{trans-CH}_3\text{CH}=\text{CHCH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHCH}=\text{C}=\text{CH}_2 + \text{H}_2$ (a)							
$\rightarrow \text{cis-CH}_3\text{CH}=\text{CHCH}=\text{CH}_2$ (b)							
1,3-Pentadiene, (E)-							
82 NGU/KIN2	EX	1002-1235	¹⁾	¹⁾	¹⁾	1	
k_a . Unimolecular thermolysis. VLPP-technique. Mass-spectrometry.							
¹⁾ Curved Arrhenius plot.							
For 1100 K the authors give:							
$k = 1.0 \times 10^{13} \exp(-32461 \pm 1007) \text{ s}^{-1}$.							
71 FRE/LAM	RN	473-517	2.00(13)	.0	26487±301	1	1.55
k_b . Thermal isomerization in a static system. Gas-chromatography.							
k is P-independent between 0.75 and 7.5 torr. Determined from the Equilibrium constant and the sum of k_b and k_{-b} .							
$(\text{CH}_3)_2\text{C}=\text{C}=\text{CH}_2 \rightarrow \text{CH}_3\text{C}=\text{C}=\text{CH}_2 + \text{CH}_3$ (a)							
$\rightarrow (\text{CH}_3)_2\text{CHC}=\text{CH}$ (b)							
1,2-Butadiene, 3-methyl-							
81 NGU/KIN ¹⁾	EX	940-1222	2.00(16)	0	37896±53	1	2.0
k_a . Thermolysis.							
81 NGU/KIN ¹⁾	EX	940-1222	1.58(13)	0	32109±503	1	3.98
k_b . Thermal isomerization.							
¹⁾ 3-Methylbuta-1,2-diene pyrolysis in a VLP-Pyrolysis system. Mass-spectrometry.							
							
Cyclopentene							
74 LEW/SAR	EX	1020-1189	2.24(13)	0	30196±679	1	1.86
M = Ar. Thermolysis behind reflected shock-waves in a single-pulse shock-tube. [Cyclopentene] = (0.25-1.0)% in Ar. P = 760 torr.							
75 CRA/ROS	EX	298	(1.52±0.12)(8)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
 $\rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2$ (a) $\rightarrow \text{cis-CH}_2=\text{CHCH}=\text{CHCH}_3$ (b) $\rightarrow \text{trans-CH}_2=\text{CHCH}=\text{CHCH}_3$ (c) $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}=\text{CH}_2$ (d) $\rightarrow$  (e)						
Cyclopropane, ethenyl- (Vinylcyclopropane)						
75 CRA/ROS k_a .	EX	298	(4.7±0.1)(8)			2
75 CRA/ROS k_b .	EX	298	(3.1±0.4)(8)			2
75 CRA/ROS k_c .	EX	298	(4.2±0.5)(8)			2
75 CRA/ROS k_d . Upper-limit k.	EX	298	≤4.0(-2)			2
75 CRA/ROS k_e .	EX	298	(3.3±0.6)(8)			2
75 CRA/ROS $k_a + k_b + k_c + k_d + k_e$. Vibrationally excited Vinylcyclopropane formed by: $^1\text{CH}_2 + \text{CH}_2=\text{CHCH}=\text{CH}_2$.	EX	298	(1.52±0.07)(9)			2
 $\rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{C}=\text{CH}_2$ (a) $\rightarrow$  (b)						
Spiropentane $\rightarrow$ Ethene + 1,2-Propadiene (a) $\rightarrow$ Cyclobutane, methylene- (b)						
72 FLO/GIB ¹⁾ k_a . P = 0.9 torr. Decomposition.	EX	664	2.41(-4)			1
72 FLO/GIB ¹⁾ k_a . P = 335 torr. Decomposition.	EX	664	4.58(-5)			1
72 FLO/GIB ¹⁾ k_a . Decomposition. RRKM Calculation.	CO	643-703	7.94(13)	0	27932	1
72 FLO/GIB ¹⁾ k_b . P = 0.9 torr. Isomerisation.	EX	664	3.98(-4)			1
72 FLO/GIB ¹⁾ k_b . P = 335 torr. Isomerisation.	EX	664	7.01(-4)			1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

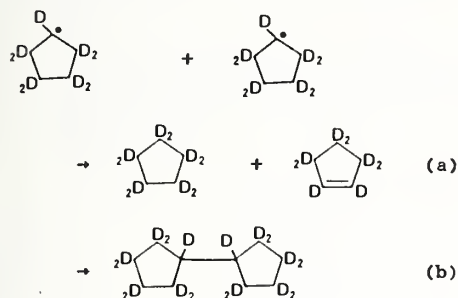
Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
¹) Pyrolysis in a static system. Gas-chromatography. Other k's, at various pressures in the (0.9-335) torr. range, with or without added CF ₂ ClCF ₂ Cl, added as inert gas, are tabulated for both, channel (a) and (b).						
[CH ₂ CH=CHCH ₂ CH ₃ = CH ₂ =CHCHCH ₂ CH ₃] → CH ₂ =CHCH=CH ₂ + CH ₃						
[2-Pentenyl = 2-Propenyl, 1-ethyl]						
81 BAL/WAL1 Oxidation of 1-Pentene in H ₂ /O ₂ mixtures in aged boric-acid-coated vessels.	ES	753	3.6(3)			1
[CH ₂ CH=CHCH ₂ CH ₃ = CH ₂ =CHCHCH ₂ CH ₃] + O ₂ → CH ₂ =CHCH=CHCH ₃ + HO ₂						
[2-Pentenyl = 2-Propenyl, 1-ethyl-] + Oxygen molecule						
80 BAL/BEN2 Oxidation of 1-Pentene and cis-2-Pentene in aged boric-acid-coated vessels. Gas-chromatography. Gas-chromatography. P(Total) = 500 torr. Same data in 81 BAL/WAL1.	ES	753	2.1(9)			2
CH ₂ CH=CHCH ₂ CH ₃ + CH ₃ CHO → CH ₃ CH ₂ CH ₂ CH=CH ₂ + CH ₃ CO (a) → cis-CH ₃ CH ₂ CH=CHCH ₃ + CH ₃ CO (b) → trans-CH ₃ CH ₂ CH=CHCH ₃ + CH ₃ CO (c)						
2-Pentenyl + Acetaldehyde						
80 RIC/MAR ¹)	ES	768	5.01(8)			2
80 RIC/MAR ¹)	ES	768	≈1.0(12)	0	6039	2
¹) k _a + k _b + k _c . Acetaldehyde pyrolysis in presence of 1,3-Butadiene, in a static system. The k's estimated by combining the present data with data found in the literature. P(1,3-Butadiene) = 20 torr. P(Acetaldehyde) = 100 torr.						
CH ₃ CH=CHCH ₂ CH ₂ → CH ₃ CH ₂ CH=CHCH ₂ (a) → CH ₃ CH ₂ CHCH=CH ₂ (b)						
3-Pentenyl						
75 STE/RAB k _a + k _b .	ES	298	2.0(9)			1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2^\dagger \rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_2\text{CH}=\text{CH}_2$ (a)						
 (b)						
4-Pentenyl $\rightarrow$ Ethene + 2-Propenyl (Allyl) (a)						
$\rightarrow$ Cyclopentyl (b)						
72 WAT/OLS ¹⁾ k_a . Decomposition.	EX	319	2.2(9)			1
72 WAT/OLS ¹⁾ k_b . Cyclization. (Intramolecular addition.)	EX	319	2.4(8)			1
¹⁾ Azo-n-propane Photolysis. $\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2^\dagger$ formed from $\text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}^\dagger$ by isomerization, with an average excess vibrational energy of 46 kcal.mol ⁻¹ . In its turn, $\text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}^\dagger$ formed by $\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}\equiv\text{CH}$. P = (90-480) torr.						
$\text{CH}_3\text{CHCH}_2\text{CH}=\text{CH}_2^\dagger \rightarrow \text{CH}_3 + \text{CH}_2=\text{CHCH}=\text{CH}_2$						
3-Butenyl, 1-methyl-						
74 CAR/TAR $\text{CH}_3\text{CHCH}_2\text{CH}=\text{CH}_2^\dagger$ formed by H + $\text{CH}_2\text{CHCH}_2\text{CH}=\text{CH}_2$.	ES	298	(3.60±0.36)(6)			1
$\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2^\dagger \rightarrow \text{CH}_3 + \text{CH}_2=\text{CHCH}=\text{CH}_2$						
3-Butenyl, 2-methyl-						
74 CAR/TAR $\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2^\dagger$ formed by isomerization from $\text{CH}_3\text{CHCH}_2\text{CH}=\text{CH}_2^\dagger$, in its turn formed by H + $\text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2$.	ES	298	(3.60±0.36)(6)			1
 + 						
$\rightarrow$  +  (a)						
$\rightarrow$  (b)						
Cyclopentyl + Cyclopentyl						
$\rightarrow$ Cyclopentane + Cyclopentene (a)						
$\rightarrow$ 1,1'-Bicyclopentyl (b)						
82 FUJ/GAE k_a/k_b . H_2O /Cyclopentane gas-phase radiolysis, in a cylindrical Pyrex vessel. Gas-chromatography.	RL	398-443	7.3(-1)	0	<500	2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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Cyclopentyl-d₈ + Cyclopentyl-d₈

→ Cyclopentane-d₁₀ + Cyclopentene-d₈ (a)

→ 1,1'-Bicyclopentyl-d₁₈ (b)

82 FUJ/GAE

RL 398-443

5.8(-1)

0

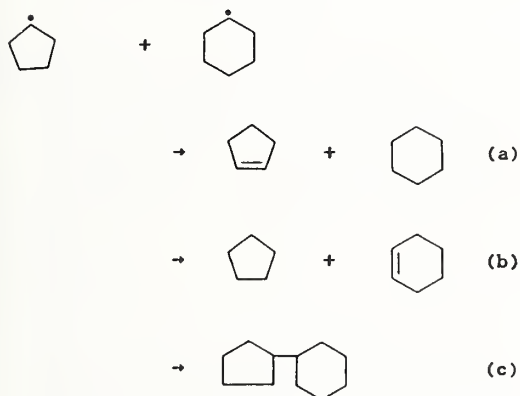
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2/2

k_a/k_b.

H₂O/Cyclopentane-d₁₀ gas-phase pyrolysis,
in a cylindrical Pyrex vessel.

Gas-chromatography.



Cyclopentyl + Cyclohexyl

→ Cyclopentene + Cyclohexane (a)

→ Cyclopentane + Cyclohexene (b)

→ Cyclohexane, cyclopentyl- (c)

82 FUJ/GAE ¹⁾

RL 398-443

3.3(-1)

0

<500

2/2

k_a/k_c.

82 FUJ/GAE ¹⁾

RL 398-443

2.8(-1)

0

<500

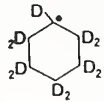
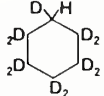
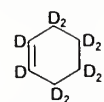
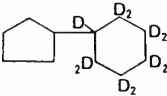
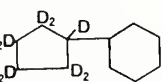
2/2

k_b/k_c.

¹⁾ H₂O/Cyclopentane/Cyclohexane gas-phase
pyrolysis, in a cylindrical Pyrex vessel.

Gas-chromatography.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
 + 						
 +  (a)						
 +  (b)						
 (c)						
Cyclopentyl + Cyclohexyl-d ₁₁						
→ Cyclopentene + Cyclohexane-d ₁₁						(a)
→ Cyclopentane-d + Cyclohexene-d ₁₀						(b)
→ Cyclohexane-d ₁₁ , cyclopentyl-						(c)
82 FUJ/GAE ¹⁾ k _a /k _c .	RL	398-443	3.5(-1)	0	<500	2/2
82 FUJ/GAE ¹⁾ k _b /k _c .	RL	398-443	2.4(-1)	0	<500	2/2
¹⁾ H ₂ O/Cyclopentane/Cyclohexane-d ₁₂ gas-phase radiolysis, in a cylindrical Pyrex vessel. Gas-chromatography.						
 + 						
 +  (a)						
 +  (b)						
 (c)						
Cyclopentyl-d ₉ + Cyclohexyl						
→ Cyclopentene-d ₈ + Cyclohexane-d						(a)
→ Cyclopentane-d ₉ + Cyclohexene						(b)
→ Cyclohexane, cyclopentyl-d ₉ -						(c)
82 FUJ/GAE ¹⁾ k _a /k _c .	RL	398-443	2.5(-1)	0	<500	2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
82 FUJ/GAE ¹⁾ k_b/k_c .	RE	398-443	2.8(-1)	0	<500	2/2
¹⁾ H ₂ O/Cyclopentane-d ₁₀ /Cyclohexane gas-phase radiolysis, in a cylindrical Pyrex vessel. Gas-chromatography.						
Cyclopentyl-d ₉ + Cyclohexyl-d ₁₁						
→ Cyclopentene-d ₈ + Cyclohexane-d ₁₂ (a)						
→ Cyclopentane-d ₁₀ + Cyclohexene-d ₁₀ (b)						
→ Cyclohexane-d ₁₁ , cyclopentyl-d ₉ (c)						
82 FUJ/GAE ¹⁾ k_a/k_c .	RL	398-443	2.8(-1)	0	<500	2/2
82 FUJ/GAE ¹⁾ k_b/k_c .	RL	398-443	2.4(-1)	0	<500	2/2
¹⁾ H ₂ O/Cyclopentane-d ₁₀ /Cyclohexane-d ₁₂ gas-phase radiolysis, in a cylindrical Pyrex vessel. Gas-chromatography.						
CH ₃ CH ₂ CH ₂ CH=CH ₂ → CH ₃ CH ₂ + CH ₂ CH=CH ₂ (a) → CH ₂ =CH ₂ + CH ₃ CH=CH ₂ (b)						
1-Pentene						
73 SHI/KIN1 k_a .	ES	753-1023	3.16(15)	0	35732	1
78 TSA2 ¹⁾ k_a .	EX	1000-1200	(1.0±0.1)(16)	0	35900	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 TSA2 ¹⁾ k _b . 1) 1-Pentene/Cyclohexene/Toluene/Ar thermolysis in in a shock-tube. k determined relative to the reaction:  → CH₂=CHCH=CH₂ + CH₃CH₃ P(Ar) ~ (1.7-5) atm. [1-Pentene] = 0.01%. [Cyclohexene] = 0.005%. [Toluene] = 1%.	EX	1000-1200	(3.16±0.95)(12)	0	28900	1	
73 SHI/KIN1 k _{overall} . CH ₃ CH ₂ CH=CHCH ₃ → CH ₃ CH=CHCH ₂ + CH ₃ (a) → any other products (b) 2-Pentene (cis-trans mixture)	EX	753-1023	1.58(12)	0	26170	1	
72 SHI/AMA k _a . 72 SHI/AMA k _{overall} .	ES	753-1003	3.16(15)	0	36236	1	
74 SPR/AKI M = NO ₂ . trans-CH ₃ CH ₂ CH=CHCH ₃ (+ M) → cis-CH ₃ CH ₂ CH=CHCH ₃ (+ M) 2-Pentene, (Z)-	EX	298-381	3.12(10)	0	5652±46'	2	1.15
74 SPR/AKI trans-CH ₃ CH ₂ CH=CHCH ₃ (+ M) → cis-CH ₃ CH ₂ CH=CHCH ₃ (+ M) 2-Pentene, (E)-	EX	298-382	5.25(10)	0	6281±44	2	1.15
CH ₃ CH ₂ C(CH ₃)=CH ₂ → CH ₃ + CH ₂ C(CH ₃)=CH ₂ 1-Butene, 2-methyl-	EX	671-722	3.98(16)	0	35732±403	1	2.51
77 TRE/WRI Limiting high-pressure k.							
CH ₃ CH ₂ C(CH ₃)=CH ₂ [†] → CH ₃ + CH ₂ C(CH ₃)=CH ₂ 1-Butene, 2-methyl-	EX	298	(5.94±0.59)(7)			1	
71 TAY/SIM ¹⁾ A7 366 nm. 71 TAY/SIM ¹⁾ At 435.8 nm.	EX	298	(3.42±0.34)(7)			1	
1) CH ₃ CH ₂ C(CH ₃)=CH ₂ [†] formed by ¹ CH ₂ + (CH ₃) ₂ C=CH ₂ . Unreported T assumed to be 287 K.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_2\text{CHCH}=\text{CH}_2 \xrightarrow{\dagger} \text{CH}_3 + \text{CH}_3\text{CHCH}=\text{CH}_2$						
1-Butene, 3-methyl-						
71 TAY/SIM ¹⁾ At 366 nm.	EX	298	(1.74±0.44)(8)			1
71 TAY/SIM ¹⁾ At 435.8 nm.	EX	298	(1.01±0.25)(8)			1
¹⁾ $(\text{CH}_3)_2$ formed by isomerization from 1,1-dimethylcyclopropane which, in its turn, was formed by $^1\text{CH}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2$. Unreported T assumed to be 298 K.						
 $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ (a)						
 $\rightarrow \text{CH}_2=\text{CH}_2 + \triangle$ (b)						
Cyclopentane						
78 TSA2 ¹⁾ k_a . Thermal isomerization.	RN	1000-1200	1.26(16)	0	42700	1
78 TSA2 ¹⁾ k_a . Thermal isomerization. k unaffected by 1-Pentene decomposition.	CO	1000-1200	6.31(15)	0	42000	1 1.58
78 TSA2 ¹⁾ k_b . Minor channel. Thermolysis.	EX	1000-1200	1.78(16)	0	47840±200	1 1.26
¹⁾ Cyclopentane/Cyclohexene/Ar thermolysis in a single-pulse shock-tube. k determined relative to the reaction:						
 $\rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CH}_3\text{CH}_3$						
[Cyclohexene] = (0.005-0.01)% [Cyclopentane] = (0.5-2.0)% P(Ar) ~ (1.7-6) atm.						
79 KAL/NAM ²⁾ k_{ref} : $\text{CH}_3\text{CH}_3 \rightarrow \text{products}$.	RL	1128-1151	(5.3±1.2)			1/1
79 KAL/NAM ²⁾ k_{ref} : $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{products}$.	RL	1023-1103	(6.7±1.8)(-1)			1/1
²⁾ $k_{\text{overall}}/k_{\text{ref}}$. Cyclopentane/Ethane (or Pentane) pyrolysis in a tubular reactor. Average ratios.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{H}_3\text{C} \begin{array}{c} \uparrow \\ \diagup \quad \diagdown \\ \text{CH}_2 \end{array} \text{CH}_3 \rightarrow \text{H}_3\text{C} \begin{array}{c} \uparrow \\ \diagdown \quad \diagup \\ \text{CH}_2 \end{array} \text{CH}_3 \quad (\text{a})$ $\rightarrow \text{cis-CH}_3\text{CH=CHCH}_2\text{CH}_3^\dagger \quad (\text{b})$ $\rightarrow \text{trans-CH}_3\text{CH=CHCH}_2\text{CH}_3^\dagger \quad (\text{c})$ $\rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2^\dagger \quad (\text{d})$ $\rightarrow \text{CH}_3\text{CH=C}(\text{CH}_3)_2^\dagger \quad (\text{e})$ Cyclopropane, 1,2-dimethyl-, cis- 72 GRO/HAS ¹⁾ k_a . 72 GRO/HAS ¹⁾ $k_a/(k_b + k_c + k_d + k_e)$. 72 GRO/HAS ¹⁾ $k_b + k_c + k_d + k_e$. ¹⁾ cis-1,2-Dimethylcyclopropane (Vibrationally excited) formed by $^1\text{CH}_2 + \text{cis-CH}_2\text{CH=CHCH}_3$.	EX	298	(5.74±0.18)(8)			1
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3^\dagger$ Pentyl 71 WAT k_{ref} : $\text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_2=\text{CHCH}_3$ Estimated ratio. 71 WAT/LAW ¹⁾ 71 WAT/LAW ¹⁾ ¹⁾ $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2^\dagger$ formed by the Azo-n-propane Photolysis.	ES	297-435	3.3(8)	0	7599	1
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2^\dagger \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3^\dagger$ Pentyl 71 WAT ¹⁾ k_{ref} : $\text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_2=\text{CHCH}_3$ Estimated ratio. 71 WAT/LAW ¹⁾ 71 WAT/LAW ¹⁾ ¹⁾ $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2^\dagger$ formed by the Azo-n-propane Photolysis.	RL	298	8.2			1/1
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 + \text{O}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH=CH}_2 + \text{HO}_2$ Pentyl + Oxygen molecule 80 BAL/BEN1 Pentane oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) ~ 500 torr.	EX	330 373	3.3(6) 8.8(6)			1 1
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 + \text{O}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH=CH}_2 + \text{HO}_2$ Pentyl + Oxygen molecule 80 BAL/BEN1 Pentane oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) ~ 500 torr.	ES	753	2.9(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_3(\text{CH}_2)_8\text{CH}_3$ (b)						
Pentyl						
71 WAT ¹⁾	RL	298	1.4(-1)			2/2
71 WAT/LAW ¹⁾	RL	330	1.5(-1)			2/2
¹⁾ k_a/k_b . Azo-n-propane Photolysis.						
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{N}=\text{NCH}_3$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + (\cdot\text{C}_5\text{H}_{10})\text{N}=\text{NCH}_3$						
Pentyl + Diazene, methylpentyl-						
71 WAT	ES	297-435	4.2(11)	0	3926	2
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2$						
Butyl, 1-methyl-						
80 BAL/BEN1 Pentane oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) ~500 torr.	ES	753	2.3(5)			1
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3^\dagger \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2$						
Butyl, 1-methyl-						
71 WAT/LAW Azo-n-propane Photolysis. $\text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3^\dagger$ formed by isomerization from $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2^\dagger$, in its turn formed by $\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_2=\text{CH}_2$.	ES	330	3.0(6)			1
78 WIE/COL ¹⁾ At 7.1 eV.	EX	298	(4.4±0.5)(6)			1
78 WIE/COL ¹⁾ At 7.6 eV.	EX	298	(1.1±0.1)(7)			1
¹⁾ Photolysis in a static system. $\text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3^\dagger$ formed by $\text{H} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$. Gas-chromatography.						
$\text{CD}_3\text{CD}_2\text{CD}_2\text{CD}_3^\dagger \rightarrow \text{CD}_3\text{CD}_2 + \text{CD}_3\text{CD}=\text{CD}_2$						
Butyl-1,2,2,3,3,4,4,4-d ₈ , 1-methyl-d ₃						
78 WIE/COL ¹⁾ At 7.1 eV.	EX	298	(1.2±0.2)(6)			1
78 WIE/COL ¹⁾ At 7.6 eV.	EX	298	(2.9±0.3)(6)			1
¹⁾ Photolysis in a static system. $\text{CD}_3\text{CD}_2\text{CD}_2\text{CD}_3^\dagger$ formed by $\text{D} + \text{CD}_3\text{CD}_2\text{CD}_2\text{CD}=\text{CD}_2$. Gas-chromatography.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃CH₂CH₂CHCH₃ + O₂							
→ CH ₃ CH ₂ CH ₂ CH=CH ₂ + HO ₂ (a)							
→ cis-CH ₃ CH ₂ CH=CHCH ₃ + HO ₂ (b)							
→ trans-CH ₃ CH ₂ CH=CHCH ₃ + HO ₂ (c)							
Butyl, 1-methyl- + Oxygen molecule							
80 BAL/BEN1	RL	753	2.3				2/2
(k _b + k _c)/k _a . Oxidation in aged boric-acid-coated Gas-chromatography. Estimated ratio. P(Total) ~ 500 torr.							
CH₃CH₂CH₂CHCH₃ + CH₃CH₂CH₂CH₂CH₂							
→ CH ₃ (CH ₂) ₂ CH(CH ₃)(CH ₂) ₄ CH ₃ (a)							
→ CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ + CH ₃ CH ₂ CH ₂ CH=CH ₂ (b)							
→ CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ + CH ₃ CH ₂ CH=CHCH ₃ (c)							
Butyl, 1-methyl- + Pentyl							
71 WAT	RL	298	1.41				2/2
(k _a + k _b + k _c)/k _a .							
CH₃CH₂CHCH₂CH₃ → CH₃CH₂CH=CH₂ + CH₃							
Propyl, 1-ethyl-							
80 BAL/BEN1	ES	753	1.57(5)				1
Pentane oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) ~ 500 torr.							
CH₃CH₂CHCH₂CH₃ + O₂ → cis-CH₃CH₂CH=CHCH₃ + HO₂ (a)							
→ trans-CH₃CH₂CH=CHCH₃ + HO₂ (b)							
Propyl, 1-ethyl- + Oxygen molecule							
80 BAL/BEN1 ¹⁾	RL	753	(1.55±0.09)(6)				2/1
(k _a + k _b)/k _{ref} . k _{ref} : CH ₃ CH ₂ CHCH ₂ CH ₃ → CH ₃ CH ₂ CH=CH ₂ + CH ₃							
80 BAL/BEN1 ¹⁾	ES	753	2.42(11)				2
¹⁾ Oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) ~ 500 torr.							
(CH₃)₃CCH₂ (+ M) → (CH₃)₂C=CH₂ + CH₃ (+ M)							
Propyl, 2,2-dimethyl-							
75 SZI/MAR1	ES	512-571	2.0(13)	0	14997±1007	1	6.31
77 MUL/BAR	ES	~753	≈1.0(13)	0	15098	1	
Pyrolysis in a static reactor.							
79 SZI/MAR	RN	512-571	2.51(13)	0	14915±962	1	6.31
Pyrolysis of Neopentane in presence of Azoisopropane. P(Total) = (15-300) torr.							

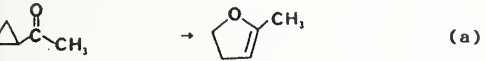
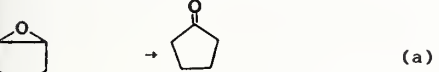
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
72 FUR/LAI2 ¹) Limiting high-pressure k.	RN	503-608	2.5(13)	0	14595±252	1	
72 FUR/LAI2 ¹) Limiting low-pressure k.	RN	503-608	5.8(10)	0	8606±252	2	
¹) Hg-photosensitized decomposition of Neopentane. P = (10-280) torr.							
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{products}$							
Pentane							
79 KAL/NAM Pyrolysis of mixtures of Cyclopentane with Ethane and Pentane. k_{ref} : $\text{CH}_3\text{CH}_3 \rightarrow \text{products}$.	RL	1103	6.2			1/1	
79 ZYC/BAC Pyrolysis in a tubular reactor. P = 1 atm.	EX	1000-1120	6.2(11)	0	26875±201	1	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3^\dagger \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2$ (b)							
Pentane							
72 HAS/JOH ¹) $k_a + k_b$. P = 0.066 torr.	EX	298	(1.5±0.1)(6)			1	
72 HAS/JOH ¹) $k_a + k_b$. P = 0.079 torr.	EX	298	(1.8±0.1)(6)			1	
¹) $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3^\dagger$ formed by $^1\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$.							
$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3^\dagger \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}_2\text{CHCH}_3$ (a) $\rightarrow \text{CH}_3 + (\text{CH}_3)_2\text{CHCH}_2$ (b) $\rightarrow \text{CH}_3\text{CH}_2 + (\text{CH}_3)_2\text{CH}$ (c)							
Butane, 2-methyl- (Isopentane)							
72 HAS/JOH ¹) $k_a + k_b + k_c$. At 366 nm.	EX	298	(3.1±0.2)(6)			1	
72 HAS/JOH ¹) $k_a + k_b + k_c$. At 435.8 nm.	EX	298	(1.6±0.1)(6)			1	
¹) $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3^\dagger$ formed by $^1\text{CH}_2 + (\text{CH}_3)_3\text{CH}$.							
72 HAS/JOH ²) $k_a + k_b + k_c$. At 366 nm.	EX	298	(2.8±0.1)(6)			1	
72 HAS/JOH ²) $k_a + k_b + k_c$. At 435.8 nm.	EX	298	(2.2±0.1)(6)			1	
²) $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3^\dagger$ formed by $^1\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$(\text{CH}_3)_4\text{C} \rightarrow (\text{CH}_3)_3\text{C} + \text{CH}_3$							
Propane, 2,2-dimethyl- (Neopentane)							
71 BAR/DZI	ES	723-803	6.31(16)	0	41268	1	
73 PAC	EX	793-953	5.01(17)	0	42821±722	1	2.0
76 BRA/WES1	DE	1030-1300	3.3(16)	0	40416	1	1.29
Computer-fit of experimental data.							
76 MAR/PUR	EX	756-845	1.26(16)	0	39694±1804	1	10.0
78 MAR/COM	EX	703-743	3.98(17)	0	42275	1	
Stirred flow-reactor pyrolysis.							
P(Neopentane) = 50 torr.							
78 PAC/WIM	EX	821	(2.4±0.1)(-5)			1	
Neopentane flow-pyrolysis.							
P = 7.6 torr.							
79 BAL/LEW2	EX	1000-1260	2.00(17)	0	40664	1	
VLP-Pyrolysis. Mass spectrometry.							
80 PAC/WIM1	EX	823	(1.7±0.1)(-5)			1	
Pyrolysis of Neopentane in a flow reactor.							
Gas-chromatography.							
P = (4-335) torr.							
81 PRA/ROG	EX	945-1016	1.38(15)	0	40051	1	
Pyrolysis in a wall-less reactor, in Ar.							
P(Ar) = 600 torr.							
$\text{CH}_3\text{C}\equiv\text{CCH}_2\text{COOH} \rightarrow \text{CH}_3\text{CH}=\text{C}=\text{CH}_2 + \text{CO}_2$							
3-Pentynoic acid							
76 BIG/WEA1	EX	500	3.36(-6)			1	
76 BIG/WEA1	EX	662	4.43(-2)			1	
76 BIG/WEA1	EX	500-663	2.47(11)	0	19438±758	1	
A and B recalculated from the reported data.							
$\text{CH}_3\text{C}\equiv\text{CCH}_2\text{COOD} \rightarrow \text{CH}_3\text{CD}=\text{C}=\text{CH}_2 + \text{CO}_2$							
3-Pentynoic acid-d							
76 BIG/WEA1	EX	630	3.30(-3)			1	
$\text{CH}_2=\text{C}=\text{CHCH}_2\text{COOH} \rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CO}_2$							
3,4-Pentadienoic acid							
76 BIG/WEA2	EX	500	3.35(-7)			1	
76 BIG/WEA2	EX	630	1.35(-3)			1	
76 BIG/WEA2	EX	500-715	1.05(11)	0	20152±758	1	2.6
A and B recalculated from the reported data.							

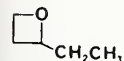
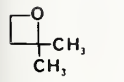
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 Furan, 2,3-dihydro-5-methyl- → Ethanone, 1-cyclopropyl- 73 COC/EGG Pyrolysis. P-independent for P > 4 torr.	EX	672-731	7.07(14)	0	28989±349	1	1.66
 → cis-CH ₃ C(O)CH=CHCH ₃ (b) → trans-CH ₃ C(O)CH=CHCH ₃ (c) → CH ₃ C(O)CH ₂ CH=CH ₂ (d) Ethanone, 1-cyclopropyl- → Furan, 2,3-dihydro-5-methyl- (a) → 3-Penten-2-one, (Z)- (b) → 3-Penten-2-one, (E)- (c) → 4-Penten-2-one (d)	EX	672-731	7.76(13)	0	27810±349	1	1.7
73 COC/EGG ¹⁾ k _a .	ES	672-731	6.31(13)	0	28989	1	
73 COC/EGG ¹⁾ k _b .	ES	672-731	1.58(13)	0	28989	1	
73 COC/EGG ¹⁾ k _c .	ES	672-731	3.98(14)	0	30071	1	
73 COC/EGG ¹⁾ k _d .	EX	672-731	2.51(14)	0	29289±505	1	2.14
73 COC/EGG ¹⁾ k _b + k _c + k _d .							
¹⁾ Thermal isomerization. P-independent for P > 4 torr.							
 → 2-Cyclopenten-1-ol (b) → CH ₂ =CHCHO + CH ₂ =CH ₂ (c) → other products (d)							
6-Oxabicyclo[3.1.0]hexane → Cyclopentanone (a)							
→ 2-Cyclopenten-1-ol (b)							
→ 2-Propenal (Acrolein) + Ethene (c)							
→ other products (d)							
74 FLO/PEN1 ¹⁾ k _a .	EX	670-742	1.45(14)	0	28916±180	1	1.29

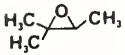
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
74 FLO/PEN1 ¹⁾ k _b .	EX	670-742	3.63(13)	0	29133±265	1	1.45
74 FLO/PEN1 ¹⁾ k _c . The reactant might isomerize to Cyclobutanecarboxaldehyde before decomposing.	EX	670-742	4.07(14)	0	32296±433	1	1.82
74 FLO/PEN1 ¹⁾ k _a + k _b + k _c + k _d .	EX	670-742	2.00(14)	0	28989±108	1	1.17
¹⁾ Thermolysis. P = (1-28) torr.							
 CH₃CH=CHCH₂COOH → CH₃CH=CHCH₃ + CO₂ 3-Pentenoic acid							
76 BIG/WEA1	EX	500	2.01(-7)				1
76 BIG/WEA1	EX	693	1.05(-3)				1
76 BIG/WEA1	EX	500-720	2.34(11)	0	20814±782	1	
A and B recalculated from the reported data.							
 CH₃C(O)C(O)CH₂CH₃ → CH₃CO + CH₃CH₂CO (a) → any other products (b)							
2,3-Pentanedione							
74 SCH/KNO	EX	362-398	≈7.94(16)	0	33971±1459	1	10.0
k _a . Order of magnitude estimate: k _a ~ 0.1k _b .							
74 SCH/KNO	EX	362-398	7.94(17)	0	33971±1459	1	10.0
k _{overall} .							
 CH₂=C(CH₃)CH₂COOH → (CH₃)₂C=CH₂ + CO₂ 3-Butenoic acid, 3-methyl- → 1-Propene, 2-methyl- + Carbon dioxide							
77 BIG/WEA ¹⁾ k/k _{ref} .	RL	500	2.03(1)				1/1
k _{ref} : CH ₂ =C(CH ₃)CH ₂ COOH → CH ₂ =C(CH ₃) ₂ + CO ₂							
77 BIG/WEA ¹⁾	EX	500	3.05(-5)				1
¹⁾ Pyrolysis in a flow-reactor. Gas-chromatography.							
 △CH₃COOH → CH₃CH₂CH=CH₂ + CO₂ (a) = (b) → (CH ₃) ₂ C=CH ₂ + CO ₂ (c)							
Cyclopropaneacetic acid → 1-Butene + Carbon dioxide (a) = (b) → 1-Propene, 2-methyl- + Carbon dioxide (c)							
80 BIG/FET ¹⁾ k _a = k _b .	EX	725	1.0(-3)				1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 BIG/FET ¹⁾ k _c . Upper-limit k.	EX	725	<4.0(-5)			1
80 BIG/FET ¹⁾ k _a + k _b + k _c .	EX	725	2.0(-3)			1
80 BIG/FET ¹⁾ k _a + k _b + k _c . A and B recalculated from the reported data.	EX	750-820	2.18(11)	0	23434±722	1
¹⁾ Pyrolysis in a flow-reactor. NMR-spectrometry.						
<chem>CH3CH2OCH2CH=CH2 -> CH3CHO + CH3CH=CH2</chem> 1-Propene, 3-ethoxy-						
74 EGG/VIT2	EX	560-648	6.92(11)	0	21928±388	1 1.95
<chem>CH3CH2CH2OCH=CH2 -> CH3CH=CH2 + CH3CHO</chem> Propane, 1-(ethenyloxy)-						
74 BAM	EX	653-708	1.32(11)	0	21399±204	1 1.35
Pyrolysis in a static system. Gas-chromatography.						
 → HCHO + <chem>CH3CH2CH=CH2</chem> (a)						
→ <chem>CH3CH2CHO</chem> + <chem>CH2CH2</chem> (b)						
Oxetane, 2-ethyl- → Formaldehyde + 1-Butene (a)						
→ Propanal + Ethene (b)						
77 CLA/HOL k _a + k _b . Pyrolysis. P = (0.45-32) torr.	EX	699-752	2.95(14)	0	29652±437	1 1.91
 → HCHO + <chem>(CH3)2C=CH2</chem> (a)						
→ <chem>(CH3)2CO</chem> + <chem>CH2=CH2</chem> (b)						
Oxetane, 2,2-dimethyl-						
82 HAM/HOL ¹⁾ k _a .	EX	675-744	3.02(13)	0	26715±349	1 1.78
82 HAM/HOL ¹⁾ k _b .	EX	675-744	3.63(15)	0	32549±529	1 2.19
82 HAM/HOL ¹⁾ k _a + k _b .	EX	675-744	6.03(13)	0	27184±325	1 1.74
¹⁾ Pyrolysis. Vacuum-system. P = (7.2-9.2) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 $\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CHO}$ (a) $\rightarrow \text{cis-CH}_3\text{CH}=\text{CHCH}_3 + \text{HCHO}$ (b) $\rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}_3 + \text{HCHO}$ (c)							
Oxetane, 2,3-dimethyl-, cis-							
$\rightarrow$ 1-Propene + Acetaldehyde (a)							
$\rightarrow$ 2-Butene, (Z)- + Formaldehyde (b)							
$\rightarrow$ 2-Butene, (E)- + Formaldehyde (c)							
74 HOL/SCO ¹⁾ k _a .	EX	688-756	5.01(15)	0	31815±312	1	1.69
74 HOL/SCO ¹⁾ k _b + k _c .	EX	688-756	1.74(15)	0	31451±360	1	1.78
¹⁾ Pyrolysis. High-vacuum system. P ₀ = (2-32) torr.							
 $\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CHO}$ (a) $\rightarrow \text{cis-CH}_3\text{CH}=\text{CHCH}_3 + \text{HCHO}$ (b) $\rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}_3 + \text{HCHO}$ (c)							
Oxetane, 2,3-dimethyl-, trans-							
$\rightarrow$ 1-Propene + Acetaldehyde (a)							
$\rightarrow$ 2-Butene, (Z)- + Formaldehyde (b)							
$\rightarrow$ 2-Butene, (E)- + Formaldehyde (c)							
74 HOL/SCO k _a .	EX	688-756	8.13(15)	0	32537±334	1	1.78
74 HOL/SCO k _b + k _c .	EX	688-756	3.09(15)	0	32046±375	1	1.82
¹⁾ Pyrolysis. High-vacuum system. P ₀ = (2-32) torr.							
 $\rightarrow (\text{CH}_3)_3\text{CCHO}$ (a) $\rightarrow (\text{CH}_3)_2\text{CHC}(\text{O})\text{CH}_3$ (b) $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{OCH}_2\text{CH}_3$ (c) $\rightarrow (\text{CH}_3)_2\text{C}(\text{OH})\text{CH}=\text{CH}_2$ (d) $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}(\text{OH})\text{CH}_3$ (e)							
Oxirane, trimethyl-							
$\rightarrow$ Propanal, 2,2-dimethyl- (a)							
$\rightarrow$ 2-Butanone, 3-methyl- (b)							
$\rightarrow$ 1-Propene, 2-ethoxy- (c)							
$\rightarrow$ 3-Buten-2-ol, 2-methyl- (d)							
$\rightarrow$ 3-Buten-2-ol, 3-methyl- (e)							
75 FLO/OEZ ¹⁾ k _a .	EX	665-715	1.07(13)	0	27208±421	1	1.82
75 FLO/OEZ ¹⁾ k _b .	EX	665-715	1.12(13)	0	27052±601	1	2.40

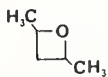
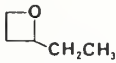
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 FLO/OEZ ¹⁾ k _c .	EX	665-715	1.51(13)	0	27738±457	1	1.95
75 FLO/OEZ ¹⁾ k _d .	EX	665-715	1.02(12)	0	27533±373	1	1.70
75 FLO/OEZ ¹⁾ k _e .	EX	665-715	8.71(11)	0	25681±986	1	4.17
75 FLO/OEZ ¹⁾ k _a + k _b + k _c + k _d + k _e .	EX	665-715	6.31(13)	0	27473±505	1	2.09
¹⁾ Thermolysis. Static system. P = (1.5-27) torr.							
<chem>CH3OCH2CH2OCH=CH2 -> CH3OCH=CH2 + CH3CHO</chem> Ethene, (2-methoxyethoxy)-							
74 BAM Pyrolysis in a static system. Gas-chromatography.	EX	653-708	1.38(11)	0	22241±144	1	1.23
<chem>CH3C(O)OCH2CH2CH3 -> CH3COOH + CH3CH=CH2</chem> Acetic acid propyl ester (n-Propyl acetate)							
76 DEB/TAY	EX	650-700	4.47(12)	0	24409	1	
<chem>CH3C(O)OCH(CH3)2 -> CH3COOH + CH3CH=CH2</chem> Acetic acid 1-methylethyl ester (i-Propyl acetate)							
75 TAY Pyrolysis. CH ₃ COOH decomposes fast to CO ₂ + CH ₄ .	EX	609-657	1.58(13)	0	23020±302	1	1.58
77 SMI/MUT	EX	651	(5.93±0.17)(-3)			1	
78 TAY Pyrolysis in a stainless-steel reactor.	EX	609-668	1.62(13)	0	22994	1	
82 MCM/LEW Ethyl acetate/Isopropyl acetate/Isobutyl bromide/SF ₆ /CO ₂ laser-powered homogeneous pyrolysis. P(Acetate, or Bromide) ~1.0 torr. P(SF ₆) = 4 torr. P(CO ₂) = 93 torr.	EX	950-1000	5.01(12)	0	22496	1	
<chem>CH3CH2C(O)OHCH2CH3 -> CH3CH2COOH + CH2=CH2</chem> Propanoic acid ethyl ester							
76 BAR/COC Reflected shock-waves in single-pulse shock-tubes. Curved Arrhenius plot above 1100 K.	EX	919-1220	5.25(12)	0	24418	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{CH}_2\text{OC(O)OCH}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{CH}_2 + \text{CO}_2 + \text{CH}_3\text{CH}_2\text{OH}$							
Carbonic acid diethyl ester (Diethyl carbonate)							
72 BIG/WRE1 ¹⁾ Sealed-tube pyrolysis.	EX	554-594	1.43(13)	0	23352	1	
72 BIG/WRE1 ¹⁾ Flow-tube pyrolysis.	EX	700	(7.40±0.22)(-2)			1	
72 BIG/WRE1 ¹⁾ Flow-tube pyrolysis. The A-factor recalculated from reported data.	EX	663-708	(4.05±0.12)(13)	0	23754	1	
¹⁾ Diethyl carbonate pyrolysis.							
76 CRO/HUN	EX	584-663	1.15(13)	0	23456	1	
$\text{CH}_3\text{C(O)OCH}_2\text{CH}_2\text{OCH}_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHOCH}_3$							
Ethanol, 2-(methoxy)-, acetate							
76 DEB/TAY	EX	650-700	7.94(12)	0	25767	1	
80 CHU/MAR Gas phase pyrolysis in a static system. Gas-chromatography. P = (63-207) torr.	EX	592-723	1.09(12)	0	24502±352	1	1.74
$\text{HOCH}_2\text{C(O)OCH}(\text{CH}_3)_2 \rightarrow \text{HOCH}_2\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$							
Acetic acid, hydroxy-, 1-methylethyl ester							
77 CHU/MAR	EX	563-623	3.63(12)	0	21641±352	1	1.91
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{O} \rightarrow \text{CH}_3\text{CH}_2 + (\text{CH}_3)_2\text{CO}$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{COCH}_3 + \text{CH}_3$ (b)							
Propoxy, 1,1-dimethyl-							
78 BAT/ISL1 ¹⁾ k_a .	EX	433-463	5.01(14)	0	7197±503	1	1.58
78 BAT/ISL1 ¹⁾ k_a/k_b .	RL	433	(8.0±0.5)(1)			1/1	
79 BAT ¹⁾ k_a .	EX	393-433	6.31(14)	0	6945±500	1	3.16
78 BAT/ISL1 ¹⁾ k_b .	RN	433	1.0(15)	0	9411	1	
¹⁾ Pyrolysis in a static system. Gas-chromatography.							
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{O} + \text{NO} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{ONO}$							
Propoxy, 1,1-dimethyl- + Nitrogen oxide (NO)							
78 BAT/ISL1 Pyrolysis in a static system. Gas-chromatography. Calculated from $k_1 = k_{-1}K$.	DE	393-428	3.16(13)	0	0	2	1.58

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_3\text{CCH}_2\text{OO} \rightarrow (\text{CH}_3)_2\text{C}(\text{CH}_2\text{OOH})\text{CH}_2$ (a) $\rightarrow (\text{CH}_3)_2\text{CCH}_2(\text{O})\text{OCH}_3$ (b)						
Propyldioxy, 2,2-dimethyl-						
75 BAK/BAL1	ES	753	1.85(4)			1
k_a .						
75 BAK/BAL1	ES	298-753	1.26(12)	0	13588	1
k_a .						
75 BAK/BAL1	ES	753	$\leq 1.6(3)$			1
k_b . Upper-limit k.						
$\text{CH}_3\text{CH}(\text{OOH})\text{CH}_2\text{CHCH}_3 \rightarrow$  $+ \text{OH}$						
Butyl, 3-hydroperoxy-1-methyl-						
$\rightarrow$ Oxetane, 2,4-dimethyl- + Hydroxyl						
80 BAL/BEN1	ES	753	1.0(6)			1
Pentane oxidation in aged boric-acid-coated vessels.						
Gas-chromatography.						
P(Total) ~ 500 torr.						
$\text{HOOCCH}_2\text{CH}_2\text{CHCH}_2\text{CH}_3 \rightarrow$  $+ \text{OH}$						
Propyl, 3-hydroperoxy-1-ethyl,						
$\rightarrow$ Oxetane, 2-ethyl- + Hydroxyl						
80 BAL/BEN1	ES	753	1.0(6)			1
Pentane oxidation in aged boric-acid-coated vessels.						
Gas-chromatography.						
P(Total) ~ 500 torr.						
$(\text{CH}_3)_2\text{C}(\text{CH}_2\text{OOH})\text{CH}_2 \rightarrow$  $+ \text{OH}$						
Propyl, 2-methyl-2-hydroperoxymethyl-						
$\rightarrow$ Oxetane, 3,3-dimethyl-						
75 BAK/BAL1	ES	753	1.0(6)			1 2.0
75 BAK/BAL1	ES	298-753	6.31(11)	0	10065	1 2.0
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OO} \rightarrow \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OOH}$ (a) $\rightarrow \text{CH}_3\text{CHCH}_2\text{CH}_2\text{CH}_2\text{OOH}$ (b) $\rightarrow \text{CH}_3\text{CH}_2\text{CHCH}_2\text{CH}_2\text{OOH}$ (c)						
Pentyldioxy						
80 BAL/BEN1 ¹⁾	RL	753	(3.1±0.4)(-1)			1/1
k_a/k_c .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
80 BAL/BEN1 ¹⁾ k _a .	RN	753	9.3(4)			1	
80 BAL/BEN1 ¹⁾ k _b /k _c .	RL	753	(2.2±0.3)			1/1	
80 BAL/BEN1 ¹⁾ k _b .	RN	753	6.6(5)			1	
80 BAL/BEN1 ¹⁾ k _c .	ES	753	3.0(5)			1	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{OO}\cdot)\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CHCH}(\text{OOH})\text{CH}_3$ (a) $\rightarrow \text{CH}_3\text{CHCH}_2\text{CH}(\text{OOH})\text{CH}_3$ (b)							
Butyldioxy, 1-methyl-							
80 BAL/BEN1 ¹⁾ k _a /k _b .	RL	753	(6.3±2.5)			1/1	
80 BAL/BEN1 ¹⁾ k _a .	RN	753	4.7(5)			1	
80 BAL/BEN1 ¹⁾ k _b .	ES	753	3.0(5)			1	
¹⁾ Pentane oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) ~ 500 torr.							
$\text{CH}_3\text{CH}(\text{OOH})\text{CH}_2\text{CH}(\text{OO}\cdot)\text{CH}_3 \rightarrow \text{CH}_3\text{CHO} + \text{CH}_3\text{CHO} + \text{HCHO} + \text{OH}$							
Butyldioxy, 3-hydroperoxy-1-methyl-							
80 BAL/BEN1 Pentane oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) ~ 500 torr.	ES	753	5.0(5)			1	
$\text{CH}_3\text{CH}_2\text{CH}(\text{OO}\cdot)\text{CH}_2\text{CH}_2\text{OOH} \rightarrow \text{CH}_3\text{CH}_2\text{CHO} + \text{HCHO} + \text{HCHO} + \text{OH}$							
Propyldioxy, 3-hydroperoxy-1-ethyl-							
80 BAL/BEN1 Pentane oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) = ~ 500 torr.	ES	753	8.0(5)			1	
$(\text{CH}_3)_2\text{C}(\text{CH}_2\text{OOH})\text{CH}_2\text{OO} \rightarrow (\text{CH}_3)_2\text{CO} + 2\text{HCHO} + \text{OH}$							
Propyldioxy, 2-hydroperoxymethyl-2-methyl-							
75 BAK/BAL1	ES	753	1.5(6)			1	2.0
75 BAK/BAL1	ES	298-753	6.31(11)	0	9562	1	2.0
$(\text{CH}_3)_3\text{COCH}_3 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3\text{OH}$							
Propane, 2-methoxy-2-methyl-							
74 CHO/GOL The A and B factors are recommended for T = 800 K.	EX	780-917	7.94(13)	0	29693±503	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

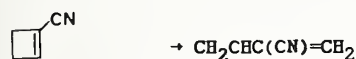
Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{COSCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{COS} + \text{CH}_3\text{CH}=\text{CH}_2$ Ethanethioic acid S-(1-methylethyl) ester							
72 OEL/TIN Elimination by thermolysis.	EX	723-799	1.58(13)	0	24761	1	
$\text{CH}_3\text{C}(\text{S})\text{OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{COS} + \text{CH}_3\text{CH}=\text{CH}_2$ (a) $\rightarrow \text{CH}_3\text{COSCH}(\text{CH}_3)_2$ (b) Ethanethioic acid O-(1-methylethyl) ester							
75 BIG/GAB ¹⁾ k _a . Elimination.	EX	629	5.12(-1)			1	
75 BIG/GAB ¹⁾ k _a . Elimination.	EX	563-583	7.94(12)	0	19099	1	
75 BIG/GAB ¹⁾ k _a + k _b . Overall reaction.	EX	559	1.01(-2)			1	
75 BIG/GAB ¹⁾ k _a + k _b . Overall reaction.	EX	563-583	7.08(12)	0	19099	1	
¹⁾ Flow reactor pyrolysis.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{SCH}_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHSCH}_3$ Ethanol, 2-(methylthio)-, acetate							
80 CHU/MAR Pyrolysis. Static system. P = (63-207) torr.	EX	592-723	1.86(11)	0	21531±553	1	2.45
$\text{CH}_3\text{C}(\text{O})\text{SCH}(\text{CH}_3)\text{OCH}_3 \rightarrow \text{CH}_3\text{C}(\text{S})\text{OH} + \text{CH}_2=\text{CHOCH}_3$ (a) $\rightarrow \text{CH}_3\text{COSH} + \text{CH}_2=\text{CHOCH}_3$ (b) Ethanethioic acid S-(1-methoxyethyl) ester							
72 OEL/TIN k _a + k _b . Thermolysis.	EX	583-633	1.00(13)	0	19930	1	
$\text{CH}_3\text{OC}(\text{S})\text{OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{OH} + \text{COS} + \text{CH}_3\text{CH}=\text{CH}_2$ Carbonothioic acid O-methyl O-(1-methylethyl) ester							
82 ALA/BIG ¹⁾	EX	629	1.5			1	
82 ALA/BIG ¹⁾ A and B recalculated from the reported data.	EX	500-560	1.19(11)	0	15785	1	
¹⁾ Pyrolysis in a flow reactor. IR-spectrometry. P = (2-800) torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
$\text{CH}_3\text{OC}(\text{O})\text{SCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{OH} + \text{COS} + \text{CH}_3\text{CH}=\text{CH}_2$						
Carbonothioic acid O-methyl S-(1-methylethyl) ester						
79 ALA/BIG ¹⁾	EX	629	4.6(-5)			1
79 ALA/BIG ¹⁾	EX	713-753	9.04(12)	0	25047±722	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a flow-reactor.						
IR-spectrometry.						
$(\text{CH}_3)_2\text{CHOC}(\text{O})\text{SCH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CO}_2 + \text{CH}_3\text{SH}$						
Carbonothioic acid S-methyl O-(1-methylethyl) ester						
79 ALA/BIG ¹⁾	EX	629	9.4(-3)			1
79 ALA/BIG ¹⁾	EX	820-857	7.27(11)	0	20115±1203	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a Flow-reactor.						
IR-spectrometry.						
 $\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_2=\text{CH}_2 + \text{SO}_2$						
Thiophene, tetrahydro-3-methyl-1,1-dioxide-						
(3-Methylsulfolane)						
$\rightarrow$ 1-Propene + Ethene + Sulfur dioxide						
75 COR/TSA	EX	733-798	1.3(16)	0	33200±750	1 2.51
Pyrolysis in a flow-tube reactor.						
$\text{CH}_3\text{SC}(\text{S})\text{OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{SH} + \text{COS} + \text{CH}_3\text{CH}=\text{CH}_2$						
Carbonodithioic acid S-methyl O-(1-methylethyl) ester						
82 ALA/BIG ¹⁾	EX	629	5.6(-1)			1
82 ALA/BIG ¹⁾	EX	500-550	1.39(12)	0	17950	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a flow reactor.						
IR-spectrometry.						
P = (2-800) torr.						
$\text{CH}_3\text{OC}(\text{S})\text{SCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{OH} + \text{CS}_2 + \text{CH}_3\text{CH}=\text{CH}_2$						
Carbonodithioic acid O-methyl S-(1-methylethyl) ester						
82 ALA/BIG ¹⁾	EX	629	7.9(-1)			1
82 ALA/BIG ¹⁾	EX	580-630	7.40(11)	0	20235	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a flow reactor.						
IR-spectrometry.						
P = (2-800) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k(k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
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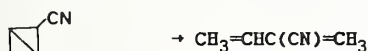


1-Cyclobutene-1-carbonitrile

→ 3-Butenenitrile, 2-methylene-

72 SAR/GAL ¹⁾	EX	463-498	2.51(13)	0	16910	1
72 SAR/GAL ¹⁾	SE	463-498	2.39(13)	0	16910	1

Average value of previous
and present data.

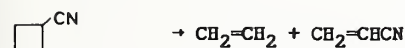
¹⁾ Thermal isomerization in a flow-reactor.
Gas-chromatography.


Bicyclo[1.1.0]butane-1-carbonitrile

→ 3-Butenenitrile, 2-methylene-

72 SAR/GAL ¹⁾	EX	726-783	7.94(13)	0	20181	1
72 SAR/GAL ¹⁾	SE	726-783	8.43(13)	0	20181	1

Average value of previous
and present data.

¹⁾ Thermal isomerization in a flow-reactor.
Gas-chromatography.


Cyclobutanecarbonitrile → Ethene + 2-Propenenitrile

72 SAR/GAL ¹⁾	EX	726-783	2.03(15)	0	28535	1
72 SAR/GAL ¹⁾	SE	726-783	3.16(15)	0	28535	1

Average value of previous
and present data.

¹⁾ Thermal isomerization in a flow-reactor.
Gas-chromatography.

75 KIN/GOD3 ²⁾	EX	833-1203	1.0(15)	0	28686±503	1
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Based on the present VLPP results
and previous high-pressure data.

75 KIN/GOD3 ²⁾	EX	833-1203	7.94(15)	0	29743±503	1
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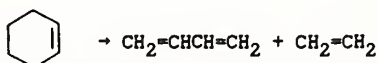
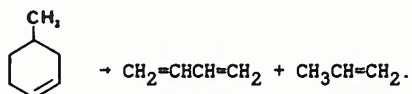
Based on combination of present
and previous VLPP data.

²⁾ VLP-Pyrolysis system.

P = (0.1-1.0) mtorr.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$(\text{CH}_3)_2\text{CHCH}_2\text{CN} \rightarrow (\text{CH}_3)_2\text{CH} + \text{CH}_2\text{CN}$							
Butanenitrile, 3-methyl-							
75 KIN/GOD2	EX	1011-1123	2.51(15)	0	36789±856	1	2.0
$(\text{CH}_3)_3\text{CCN} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{HCN}$ (a)							
$\rightarrow (\text{CH}_3)_2\text{CCN} + \text{CH}_3$ (b)							
Propanenitrile, 2,2-dimethyl-							
73 DAS/EMO	EX	838-927	1.58(12)	0	32053±247	1	1.02
k_a .							
76 KIN/GOD	EX	1023-1254	1.26(14)	0	37292±805	1	2.0
k_a .							
76 KIN/GOD	EX	1023-1254	7.94(15)	0	37695±805	1	2.0
k_b .							
$\text{CH}_3\text{CH}_2\text{N}=\text{NCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}_2 + (\text{CH}_3)_2\text{CH} + \text{N}_2$							
Diazene, ethyl-(1-methylethyl)-							
77 MAR/MAC	EX	533-593	3.16(16)	0	24779±361	1	3.16
Thermolysis in a vacuum system.							
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{NH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2 + \text{NH}_2$ (a)							
$\rightarrow \text{CH}_3\text{CH}_2 + (\text{CH}_3)_2\text{CNH}_2$ (b)							
$\rightarrow (\text{CH}_3)_2\text{C}=\text{CHCH}_3 + \text{NH}_3$ (c)							
2-Butanamine, 2-methyl- (t-Amylamine)							
78 TSA1 ¹⁾	EX	990-1200	7.94(15)	0	39700±500	1	2.0
k_a .							
78 TSA1 ¹⁾	EX	990-1200	3.16(16)	0	38500±500	1	2.0
k_b .							
78 TSA1 ¹⁾	EX	990-1200	<3.16(14)	0	37200	1	
k_c . Upper-limit k.							
¹⁾ t-Amylamine/4-Methylcyclohexene (or Hexene)/							
Toluene/Ar thermolysis in a shock-tube.							
k's deterative to either of							
the two reactions:							



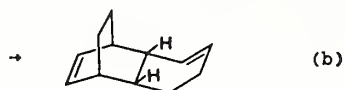
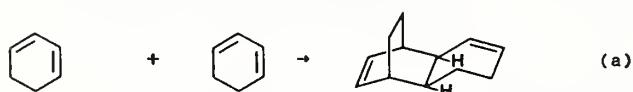
[t-Amylamine] = (0.1-0.4)%. [Cyclohexene] = 1%, or
 [4-Methylcyclohexene] = 0.025%.
 [Toluene + Argon] = 1%.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CN} \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CNCN}$							
Propanenitrile, 3-(acetyloxy)-							
80 CHU/MAR	EX	592-723	3.24(11)	0	20677±204	1	1.35
Gas phase pyrolysis in a static system.							
Gas-chromatography.							
P = (63-207) torr.							
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{ONO} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{O} + \text{NO}$							
Nitrous acid 1,1-dimethylpropyl ester (1,1-dimethylpropyl nitrite)							
78 BAT/ISL1	EX	393-428	2.00(16)	0	20280±50	1	1.26
Pyrolysis in a static system.							
Gas-liquid chromatography.							
$(\text{CH}_3)_2\text{NC}(\text{O})\text{OCH}_2\text{CH}_3 \rightarrow (\text{CH}_3)_2\text{NH} + \text{CO}_2 + \text{CH}_2=\text{CH}_2$							
Carbamic acid, dimethyl-, ethyl ester							
72 DAL/ZIO2	EX	323-333	1.26(12)	0	22315±201	1	
Thermolysis in a conventional static system.							
trans-$\text{CH}_2=\text{CHCH}=\text{CHCH}=\text{CH}_2 \rightarrow$ 							
1,3,5-Hexatriene, (E)- → 1,3-Cyclohexadiene							
73 DOE/BEA	EX	533-573	8.13(12)	0	22295±604	1	2.95
Thermal isomerization in a 12 liter Pyrex flask,							
or in a 3.5 liter corning lead-potash flask.							
Gas-chromatography.							
81 GRI/SCH	EX	555-606	(2.77±0.53)(13)	0	22914±111	1	
Thermal isomerization in an air thermostat.							
P = (2-3) torr.							
cis-$\text{CH}_3\text{CH}=\text{C}=\text{C}=\text{CHCH}_3 \rightarrow$ trans-$\text{CH}_3\text{CH}=\text{C}=\text{C}=\text{CHCH}_3$							
2,3,4-Hexatriene, (Z)-							
76 ROT/EXN	EX	373-423	1.1(13)	0	16004±151	1	
 →  + H ₂							
1,3-Cyclohexadiene → Benzene + Hydrogen molecule							
73 ALF/BEN	EX	943-1073	2.51(13)	0	29693±503	1	
VLPP in a triple-aperture quartz reactor.							
[1,3-Cyclohexadiene] = (0.01-2.0) × 10 ¹⁶ molec.cm ⁻³ .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
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1,3-Cyclohexadiene + 1,3-Cyclohexadiene

→ exo-Tricyclo[6.2.2.0^{2.7}]dodeca-3,9-diene (a)→ endo-Tricyclo[6.2.2.0^{2.7}]dodeca-3,9-diene (b)

→ Cyclohexadienyl + 2-Cyclohexen-1-yl (c)

71 DEM/HUY ¹⁾ EX 471-639 1.82(6) 0 12280±136 2 1.29
 $k_a + k_b$.

71 DEM/HUY ¹⁾ RL 471-639 1.29 0 -428±91 2/2 1.17
 k_b/k_a .

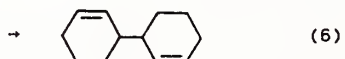
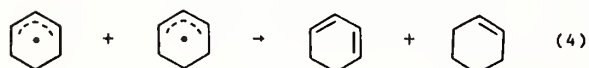
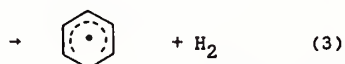
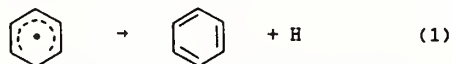
71 DEM/HUY ¹⁾ RN 471-639 9.33(8) 0 12632±252 2 1.78
 k_a .

71 DEM/HUY ¹⁾ RN 471-639 1.20(9) 0 12229±252 2 1.78
 k_b .

¹⁾ Thermal dimerization in Pyrex reaction vessel.

P = (25-630) torr.

72 DEM/HUY ²⁾ ES 512-673 2.51(13) 0 17866±503 2 2.51

 k_c . Secondary reactions for channel (c) are:

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data	T/K	k, k/k(ref),	n	B,	k, A k err.
	type		A, A/A(ref)		B-B(ref)	units factor

Cyclohexadienyl

→ Benzene + Hydrogen atom (1)

1,3-Cyclohexadiene + Hydrogen atom

→ 2-Cyclohexen-1-yl (2)

→ Cyclohexadienyl + Hydrogen molecule (3)

2-Cyclohexen-1-yl + 2-Cyclohexen-1-yl

→ 1,3-Cyclohexadiene + Cyclohexene (4)

→ Bi-2-cyclohexen-1-yl (5)

→ Cyclohexene, 3-(4-cyclohexen-1-yl) (6)

Reported rate constant ratios for the 512-673 K

T-range (all in $\text{cm}^3\text{mol}^{-1}\text{s}^{-1}$ units) are:

$$k_c k_3 / k_2 = 2.04 \times 10^{12} \exp(-17866 \pm 503) / T \quad (F = 2.51)$$

$$k_c (1 + k_3 / k_2)$$

$$= 1.35 \times 10^{13} \exp(-17866 \pm 50) / T \quad (F = 1.10)$$

based on $[\text{C}_6\text{H}_6]$, or

$$= 1.35 \times 10^{13} \exp(17866 \pm 503) / T \quad (F = 2.51)$$

by computation.

$$k_c k_4 / (k_4 + k_5 + k_6)$$

$$= 1.78 \times 10^{13} \exp(18319 \pm 554) / T \quad (F = 2.51)$$

based on $[\text{Cyclohexene}]$, or

$$= 8.32 \times 10^{12} \exp(17866 \pm 503) / T \quad (F = 2.51)$$

by computation.

$$k_c (k_5 + k_6) / (k_4 + k_5 + k_6)$$

$$= 3.31 \times 10^{12} \exp(17916 \pm 906) / T \quad (F = 4.68)$$

based on $[\text{C}_{12}\text{H}_{18}]$, or

$$= 3.02 \times 10^{12} \exp(17866 \pm 50) / T \quad (F = 2.51)$$

by computation.

$\text{C}_{12}\text{H}_{18}$ is probably Bi-2-cyclohexen-1-yl,

or 3-(4-Cyclohexen-1-yl)-cyclohexene.

2) Pyrolysis in a cylindrical Pyrex reaction vessel. Gas-chromatography.

Mass-spectrometry.

P = (10-500) torr.

All the estimated and computed rate constant ratios are based on steady-state treatment.

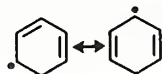
The Cyclohexadienyl radical,



formed in the channel (c) by abstraction of a H atom from a Methylene group of 1,3-Cyclohexadiene, is resonant between two forms:

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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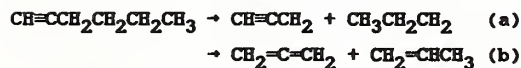
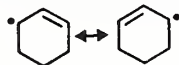


1,4-, and 1,5-Cyclohexadien-1-yl respectively.

The 2-Cyclohexen-1-yl radical,



also formed in the channel (c) by addition of a H atom to Methylidyne group adjacent to a Methylene group of 1,3-Cyclohexadiene, is resonant with its own mirror image:



1-Hexyne

78 TSA3 ¹⁾ EX 990-1200 7.94(15) 0 36300±500 1 1.58

k_a . Bond-breaking reaction.

78 TSA3 ¹⁾ EX 990-1200 5.01(12) 0 28400±1000 1 2.51

k_b . Molecular reaction.

¹⁾ 1-Hexyne/5-Methyl-1-hexyne/Toluene/Ar thermolysis in a single-pulse shock-tube. k 's determined relative to 5-Methyl-1-hexyne decomposition. [1-Hexyne] = 0.04%. [5-Methyl-1-hexyne] = 0.02%. P(Ar) ~ (2-6) atm. [Toluene] = 1%.

81 KIN2 ²⁾ EX 903-1153 7.94(15) 0 35581±1007 1 2.0

k_a . Bond-breaking reaction.

81 KIN2 ²⁾ EX 903-1153 5.01(12) 0 28385±503 1 2.51

k_b . Molecular reaction.

²⁾ 1-Hexyne thermolysis in A VLPP system.



2-Pentyne, 4-methyl-

81 KIN/NGU EX 903-1246 1.58(16) 0 37443±755 1 2.0

4-Methyl-2-pentyne thermolysis in a VLPP system.



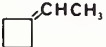
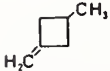
1-Butyne, 3,3-dimethyl-

77 KIN EX 933-1182 6.31(15) 0 35632±755 1 2.0

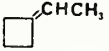
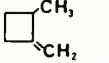
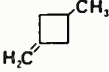
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}=\text{CH}_2 \rightarrow \text{CH}_3 + \text{CH}_2\text{CH}=\text{CHCH}=\text{CH}_2$							
1,3-Hexadiene							
80 TRE	EX	694-759	8.32(15)	0	33412±423	1	1.48
1,3-Hexadiene pyrolysis in a static system.							
Gas-chromatography.							
P = (25-200) torr.							
$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHCH}_2 + \text{CH}_2=\text{CHCH}_2$ (a)							
→ any other products (b)							
1,5-Hexadiene → 2-Propenyl (Allyl)							
71 DOE/TOS	EX	694-759	1.07(12)	0	25667±403	1	1.82
k _a . Pyrolysis in a Pyrex flask, in excess Toluene (as trapping agent for Allyl.)							
Gas-chromatography.							
76 SAK/NOH	EX	773-893	7.94(12)	0	27680	1	
k _{overall} . Flow-reactor pyrolysis. Channel (a) proposed as first step of the overall reaction.							
$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CD}_2 \rightarrow \text{CH}_2=\text{CHCH}_2\text{CD}_2\text{CH}=\text{CH}_2$							
1,5-Hexadiene-1,1-d ₂ → 1,5-Hexadiene-3,3-d ₂							
71 DOE/TOS	EX	480-531	2.29(10)	0	17262	1	
Thermal isomerization in sealed ampoules. (Cope degenerated rearrangement.) Gas-chromatography.							
$\text{cis-CH}_3\text{CH}=\text{C}(\text{CH}_3)\text{CH}=\text{CH}_2 \rightarrow \text{trans-CH}_3\text{CH}=\text{C}(\text{CH}_3)\text{CH}=\text{CH}_2$							
1,3-Pentadiene, 3-methyl-, (Z)-							
→ 1,3-Pentadiene, 3-methyl-, (E)-							
75 MAR/JEF	EX	955-1160	1.0(14)	0	27680±1007	1	2.0
Single-pulse shock-tube cis-trans isomerization in excess Ar.							
P(Ar) = (200-340) torr.							
$\text{CH}_2=\text{CHCH}(\text{CH}_3)\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2\text{CHCHCH}=\text{CH}_2 + \text{CH}_3$							
1,4-Pentadiene, 3-methyl-							
82 TRE	EX	653-716	2.29(15)	0	32733±151	1	1.26
Pyrolysis in a static system.							
Gas-chromatography.							
P = (15-200) torr.							
 → $\text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CH}_2=\text{CH}_2$							
Cyclohexene							
73 TSA1	EX	1050	1.41(15)	0	33500	1	

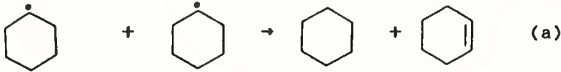
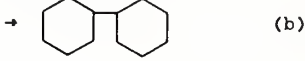
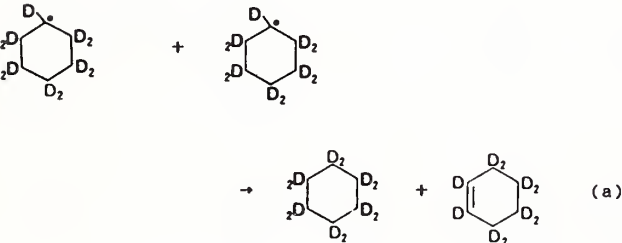
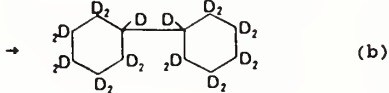
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 CHCH_3 $\rightarrow \text{CH}_3=\text{CHCH}_2 + \text{CH}_2=\text{C}=\text{CH}_2$ (a) $\rightarrow \text{CH}_3\text{CH}=\text{C}=\text{CH}_2 + \text{CH}_2=\text{CH}_2$ (b) $\rightarrow \text{CH}_3\text{CH}_2\text{C}(=\text{CH}_2)\text{CH}=\text{CH}_2$ (c) $\rightarrow$  (d)							
Cyclobutane, ethylidene-							
$\rightarrow$ 1-Propene + 1,2-Propadiene (Allene) (a)							
$\rightarrow$ 1,2-Butadiene + Ethene (b)							
$\rightarrow$ 1-Pentene, 3-methylene- (c)							
$\rightarrow$ Cyclobutane, 1-methyl-2-methylene- (d)							
71 FLO/GIB1 k_a . Decyclization and decomposition.	EX	583-697	4.90(14)	0	31520 $\pm$ 1432	1	8.51
71 FLO/GIB1 k_b . Decyclization and decomposition.	EX	583-697	1.78(15)	0	31042 $\pm$ 488	1	21.4
71 FLO/GIB1 k_c . Isomerization by decyclization.	EX	583-697	1.20(13)	0	27504 $\pm$ 2406	1	43.7
71 FLO/GIB1 k_d . Reversible rearrangement. Thermolysis in a static system. Gas-chromatography. Mass-spectrometry.	EX	583-697	8.32(13)	0	24801 $\pm$ 503	1	2.29
 $\rightarrow$ 							
Cyclobutane, 1-methyl-2-methylene-							
$\rightarrow$ Cyclobutane, ethylidene-							
71 FLO/GIB1 Thermolysis in a static system. Reversible rearrangement. Gas-chromatography. Mass-spectrometry.	EX	583-497	4.79(13)	0	24605 $\pm$ 503	1	2.29
 $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}=\text{CH}_2$							
Cyclobutane, 1-methyl-3-methylene-							
$\rightarrow$ 1,4-Pentadiene, 2-methyl-							
71 FLO/GIB2 Isomerization by decyclization. Thermolysis in a vacuum-system. Gas-chromatography. Mass-spectrometry.	EX	591-664	1.45(14)	0	26628 $\pm$ 1661	1	14.1

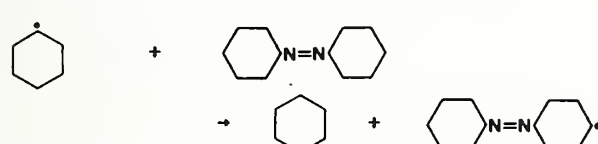
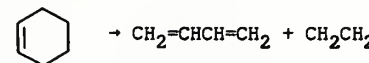
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
 $\rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2$ (a)						
$\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_2=\text{C}=\text{CH}_2$ (b)						
$\rightarrow$  (c)						
$\rightarrow$  (d)						
$\rightarrow$  (e)						
Spiropentane, methyl-						
$\rightarrow$ Ethene + 1,2-Butadiene (a)						
$\rightarrow$ 1-Propene + 1,2-Propadiene (Allene) (b)						
$\rightarrow$ Cyclobutane, ethylidene- (c)						
$\rightarrow$ Cyclobutane, 1-methyl-2-methylene- (d)						
$\rightarrow$ Cyclobutane, 1-methyl-3-methylene- (e)						
71 FLO/GIB2 ¹⁾ k _a . Decyclization and decomposition.	EX	591-664	3.02(15)	0	30003±608	1 2.63
71 FLO/GIB2 ¹⁾ k _b . Decyclization and decomposition.	EX	591-664	2.09(15)	0	30093±841	1 3.89
71 FLO/GIB2 ¹⁾ k _c . Isomerization.	EX	591-664	1.38(14)	0	27084±209	1 1.41
71 FLO/GIB2 ¹⁾ k _d . Isomerization.	EX	591-664	3.31(14)	0	27085±207	1 1.38
71 FLO/GIB2 ¹⁾ k _e . Isomerization.	EX	591-664	2.40(14)	0	27085±209	1 1.41
71 FLO/GIB2 ¹⁾ k _a + k _b + k _c + k _d + k _e . (Overall)	EX	591-664	7.59(14)	0	27084±473	1 1.41
¹⁾ Thermolysis in a static system. Gas-chromatography. Mass-spectrometry.						
CH ₂ CH ₂ CH ₂ CH ₂ CH=CH ₂ [†] $\rightarrow$ CH ₂ CH=CH ₂ + CH ₃ CH=CH ₂						
5-Hexenyl						
75 TAR ¹⁾ k _{ref} :	RL	298	8.95			1/1
(CH ₃) ₂ CCH ₂ CH ₃ [†] $\rightarrow$ (CH ₃) ₂ C=CH ₂ + CH ₃						
75 TAR ¹⁾	RN	298	3.2(7)			1
¹⁾ CH ₂ CH ₂ CH ₂ CH ₂ CH=CH ₂ [†] formed by: H + CH ₂ =CHCH ₂ CH ₂ CH=CH ₂ .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
 						
Cyclohexyl + Cyclohexyl						
→ Cyclohexane + Cyclohexene (a)						
→ 1,1'-Bicyclohexyl (b)						
74 CUR/SID k _a /k _b . Azocyclohexane photolysis in a vacuum system. Average ratio.	RL	360-460	(9.9±1.0)(-1)	0	0	2/2
79 FUJ/GAE ¹⁾ k _a /k _b . Assumed to be T-independent.	RL	343-443	(5.6±0.1)(-1)	0	0	2/2
82 FUJ/GAE ¹⁾ k _a /k _b . ¹⁾ H ₂ O/Cyclohexane gas-phase radiolysis in a Pyrex vessel. P(Total) = (50-2400) torr.	RL	398-443	5.9(-1)	0	<500	2/2
						
						
Cyclohexyl-d ₁₁ + Cyclohexyl-d ₁₁						
→ Cyclohexane-d ₁₂ + Cyclohexene-d ₁₀ (a)						
→ 1,1'-Bicyclohexyl-d ₂₂ (b)						
79 FUJ/GAE ¹⁾ k _a /k _b . Assumed to be T-independent.	RL	343-473	(3.8±0.1)(-1)	0	0	2/2
82 FUJ/GAE ¹⁾ k _a /k _b . ¹⁾ H ₂ O/Cyclohexane-d ₁₂ gas-phase radiolysis in a Pyrex vessel. P(Total) = (50-2400) torr.	RL	398-443	4.6(-1)	0	<500	2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
						
Cyclohexyl + Diazene, dicyclohexyl- (Azocyclohexane)						
74 CUR/SID Photolysis in a vacuum-system. Abstracted H assumed to be in position para to N=N group.	EX	360-460	3.98(8)	0	3322±503	2 1.26
$\text{CH}_2=\text{CH}(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2 \text{ (a)}$ $\rightarrow \text{CH}_2=\text{CHCH}_3 + \text{CH}_2=\text{CHCH}_3 \text{ (b)}$						
1-Hexene						
78 TSA5 1) k_a . Bond-breaking reaction.	EX	990-1100	7.94(15)	0	35600±150	1 1.41
78 TSA5 1) k_b . Molecular reaction.	EX	990-1100	3.98(12)	0	28900±200	1 1.58
1) 1-Hexene/Cyclohexene/Toluene/Ar thermolysis in a single-pulse shock-tube. k 's determined relative to the reaction:						
						
[1-Hexene] = 0.01%. [Toluene] = 1%. [Cyclohexene] = 0.01%. P(Ar) = 1.8 atm.						
79 KIN 2) k_a . Bond-breaking reaction.	EX	915-1153	7.94(15)	0	35632±503	1 1.58
79 KIN 2) k_b . Molecular reaction.	EX	915-1153	3.98(12)	0	29039±755	1 1.58
2) Thermolysis using a VLPP technique.						
71 MAG/IOA k_{overall} .	EX	823-923	2.0(12)	0	25667	1
$\text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{trans-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3$						
2-Hexene, (Z)-						
74 BAU/YAD Rate-ratio assumed to be T-independent. k_{ref} : $\text{cis-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}_3$	RL	1000-1150	1.0	0	0	1/1
$(\text{CH}_3)_2\text{C}(\text{CH}_3)\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3 + \text{CH}_3\text{C}(\text{CH}_3)=\text{CH}_2$						
1-Butene, 2,3-dimethyl-						
76 TSA1	ES	1080-1165	1.0(16)	0	35700	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_3\text{CCH}=\text{CH}_2 \rightarrow \text{CH}_3 + (\text{CH}_3)_2\text{CCH}=\text{CH}_2$ 1-Butene, 3,3-dimethyl-						
76 TSA1	ES	1080-1165	1.58(16)	0	35500	1
$\text{cis-CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2$ $\rightarrow \text{cis-CH}_3\text{CH}=\text{CHCH}_3 + \text{CH}_2=\text{CH}_2$ (a)						
$\rightarrow$  (b)						
$\rightarrow \text{trans-CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2$ (c)						
1,4-Butanediyl, 1,2-dimethyl-, (Z)-						
$\rightarrow$ 2-Butene, (Z)- + Ethene (a)						
$\rightarrow$ Cyclobutane, 1,2-dimethyl, cis- (b)						
$\rightarrow$ 1,4-Butanediyl, 1,2-dimethyl, (E)- (c)						
76 DER/UYE 1)	RL	579-712	1.8	0	0	1/1
k_a/k_b . Assumed to be T-independent.						
77 SCA/BAC 2)	RL	663-703	(8.73±0.73)(-1)	0	0	1/1
k_b/k_a . Average ratio.						
77 SCA/RIC 3)	RL	693	9.35(-1)			1/1
k_b/k_a .						
76 DER/UYE 1)	RL	579-712	7.0(-1)	0	0	1/1
k_b/k_c . Assumed to be T-independent.						
77 SCA/BAC 2)	RL	663-703	(2.9±0.3)(-1)	0	0	1/1
$k_b/(k_a + k_b + k_c)$. Average ratio.						
77 SCA/BAC 2)	RL	663-703	(1.36±0.10)	0	0	1/1
k_c/k_b . Average ratio.						
77 SCA/RIC 3)	RL	693	1.38			1/1
k_c/k_b .						
1) Thermolysis.						
2) Average of four rate ratios in the given T-range.						
3) Calculated ratio. Static system.						
P = 12 atm.						
$\text{trans-CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2$ $\rightarrow \text{trans-CH}_3\text{CH}=\text{CH}_3 + \text{CH}_2=\text{CH}_2$ (a)						
$\rightarrow$  (b)						
$\rightarrow \text{cis-CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2$ (c)						
1,4-Butanediyl, 1,2-dimethyl-, (E)-						
$\rightarrow$ 2-Butene, (E)- + Ethene (a)						
$\rightarrow$ Cyclobutane, 1,2-dimethyl, trans- (b)						
$\rightarrow$ 1,4-Butanediyl, 1,2-dimethyl, (Z)- (c)						
76 DER/UYE 1)	RL	579-712	1.4	0	0	1/1
k_a/k_b . Assumed to be T-independent.						

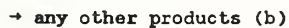
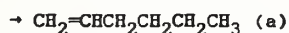
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
77 SCA/RIC ²⁾ k _a /k _{ref} . k _{ref} : cis-CH(CH ₃)CH(CH ₃)CH ₂ CH ₂ → cis-CH ₃ CH=CHCH ₃ + CH ₂ =CH ₂	RL	693	(1.66±0.1)			1/1
77 SCA/BAC ³⁾ k _b /k _a . Average ratio.	RL	663-703	(7.15±0.75)(-1)	0	0	1/1
77 SCA/RIC ²⁾ k _b /k _a .	RL	693	6.6(-1)			1/1
77 SCA/BAC ³⁾ k _b /(k _a + k _b + k _c). Average ratio.	RL	663-703	(3.23±0.15)(-1)	0	0	1/1
77 SCA/RIC ²⁾ k _b /k _{ref} . k _{ref} : cis-CH(CH ₃)CH(CH ₃)CH ₂ CH ₂ → 	RL	693	(1.0±.01)			1/1
76 DER/UYE ¹⁾ k _b /k _c . Assumed to be T-independent.	RL	579-712	1.9	0	0	1/1
77 SCA/BAC ³⁾ k _c /k _b . Average ratio.	RL	663-703	(7.00±0.25)(-1)	0	0	1/1
77 SCA/RIC ²⁾ k _c /k _b . Average ratio.	RL	693	7.15(-1)			1/1
77 SCA/BAC ³⁾ k _c /k _{ref} . Average ratio. k _{ref} : cis-CH ₃ CHCH(CH ₃)CH ₂ CH ₂ → cis-CH ₃ CH=CHCH ₃ + CH ₂ =CH ₂	RL	663-703	(1.61±0.75)(-1)	0	0	1/1

1) Thermolysis.

2) Calculated ratios. Static system. P = 12 atm.

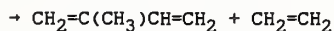
3) Average of four rate ratios in the given T-range.



Cyclohexane

78 TSA5 EX 990-1100 5.01(16) 0 44400±100 1 1.26

k_a. Cyclohexane/1-Methylcyclohexane/Ar
thermolysis in a single-pulse shock-tube.
k's determined relative to the reaction:



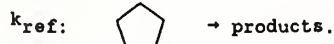
[1-Methylcyclohexene] = (0.002-0.005)%.

[Cyclohexane] = (0.4-1.0)%.

P(Ar) = (1.8-5.0) atm.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units factor	k err.
73 ILL/WEL k_{overall} .	EX	825-1005	(2.15±0.12)(14)	0	32481	1	
78 KAL/AND ¹⁾	RN	980	(2.5±0.5)(-1)			1	
78 KAL/AND ¹⁾	RN	1028	(2.1±0.1)			1	
¹⁾ k_{overall} . Cyclohexane/Hexane pyrolysis in a tubular reactor. In Hexane/Cyclohexane mixtures, the k of Cyclohexane decomposition increases when the initial [Hexane] decreases.							
79 KAL/NAM ²⁾ $k_{\text{overall}}/k_{\text{ref}}$. Average ratio. k_{ref} : $\text{CH}_3\text{CH}_3 \rightarrow \text{products}$.	RL	1033-1123	(8.4±1.3)	0	0	1/1	
79 KAL/NAM ²⁾ $k_{\text{overall}}/k_{\text{ref}}$. Average ratio. k_{ref} : $\text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{products}$.	RL	983-1133	(9.7±2.2)(-1)	0	0	1/1	
79 KAL/NAM ²⁾ $k_{\text{overall}}/k_{\text{ref}}$.	RL	1153	1.9			1/1	



Rate ratio calculated from the ratio
of other rate constants.

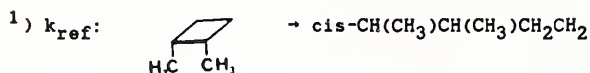
²⁾ Cyclohexane/Ethane pyrolysis in a
tubular reactor.



Cyclobutane, 1,2-dimethyl-, trans-

$\rightarrow$ 1,4-Butanediyl, 1,2-dimethyl-, (E)-

77 SCA/BAC ¹⁾ Average ratio.	RL	663-703	(5.83±0.38)(-1)	0	0	1/1	
77 SCA/RIC ¹⁾ Calculated ratio. Static system. P = 12 atm.	RL	693	(6.0±1.0)(-1)			1/1	



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{H}_3\text{C} \begin{array}{c} \diagup \text{CH}_3 \\ \triangle \\ \diagdown \text{CH}_3 \end{array}$						
→ $\text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$	(a)					
→ $\text{CH}_2=\text{CHCH}_2\text{CH}(\text{CH}_3)_2$	(b)					
→ $(\text{CH}_3)_2\text{C}=\text{CHCH}_2\text{CH}_3$	(c)					
→ cis- $\text{CH}_3\text{CH}=\text{CHCH}(\text{CH}_3)_2$	(d)					
→ trans- $\text{CH}_3\text{CH}=\text{CHCH}(\text{CH}_3)_2$	(e)					
→ $\text{CH}_2=\text{C}(\text{CH}_3)\text{CH}(\text{CH}_3)_2$	(f)					
→ $(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$	(g)					
→ other minor products	(h)					
Cyclopropane, 1,1,2-trimethyl-						
→ 1-Pentene, 2-methyl-	(a)					
→ 4-Pentene, 2-methyl-	(b)					
→ 2-Pentene, 2-methyl-	(c)					
→ 2-Pentene, 4-methyl-, (Z)-	(d)					
→ 2-Pentene, 4-methyl-, (E)-	(e)					
→ 1-Butene, 2,3-dimethyl-	(f)					
→ 2-Butene, 2,3-dimethyl-	(g)					
→ other minor products	(h)					
72 O'N/HEN ¹⁾ k _a + k _b + k _c + k _d + k _e + k _f + k _g + k _h . Overall rate constant expression.	EX	700-755	2.95(14)	0	30740±257	1
72 O'N/HEN ¹⁾ k _c .	ES	700-755	7.76(13)	0	29693	1
72 O'N/HEN ¹⁾ k _d .	ES	700-755	5.75(13)	0	30700	1
72 O'N/HEN ¹⁾ k _e .	ES	700-755	1.35(14)	0	29693	1
72 O'N/HEN ¹⁾ k _c + k _d + k _e .	ES	700-755	2.75(14)	0	29894	1
72 O'N/HEN ¹⁾ k _f .	ES	700-755	1.26(14)	0	31002	1
72 O'N/HEN ¹⁾ k _g .	ES	700-755	1.26(14)	0	31002	1
72 O'N/HEN ¹⁾ k _f + k _g .	ES	700-755	2.51(14)	0	31002	1
¹⁾ Thermolysis in a pyrex reaction-cell. Gas-chromatography. Overall rate constant determined experimentally. Rate constants for channels (a) through (g), or any combination of them, computed assuming a biradical mechanism and using transition state estimates of Arrhenius parameters (68 O'N BEN.)						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3^\dagger \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2$						
Pentyl, 1-methyl-						
75 TAR ¹⁾	RL	298	4.9(-1)			1/1
$k_{\text{ref}}: (\text{CH}_3)_2\text{CCH}_2\text{CH}_3^\dagger \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3$						
75 TAR ¹⁾	RN	298	1.8(6)			1
¹⁾ $\text{CH}_3\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ formed by: $\text{H} + \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$.						
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CH} + \text{CH}_3\text{CH}=\text{CH}_2$ (a)						
$\rightarrow \text{CH}_3 + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ (b)						
Butyl, 2,3-dimethyl-						
75 BUL/MAR	RL	667-770	(5.56±0.11)(1)	0	0	1/1
k_a/k_b .						
Static system pyrolysis. Average ratio.						
$\text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{products}$ (overall)						
Hexane						
73 ILL/WEL	EX	870-1025	(2.34±0.05)(12)	0	26522	1
P = 760 torr.						
76 RYB/YAM	EX	973-1083	3.63(10)	0	23150	1
M = Ar.						
76 RYB/YAM	EX	973-1083	1.58(10)	0	22144	1
M = D ₂ .						
78 KAL/AVD ¹⁾	RL	980	(2.0±0.4)(1)			1/1
$k_{\text{ref}}: $  $\rightarrow \text{products}.$						
78 KAL/AVD ¹⁾	RL	1028	(2.05±0.20)(1)			1/1
$k_{\text{ref}}: $  $\rightarrow \text{products}.$						
78 KAL/AVD ¹⁾	RN	980	(5.0±1.0)			1
78 KAL/AVD ¹⁾	RN	1028	(4.3±0.2)(1)			1
¹⁾ Pyrolysis in a tubular reactor. In Hexane/Cyclohexane mixtures, the k of Cyclohexane decomposition increases when the initial [Hexane] decreases.						
79 KAL/NAM ²⁾	RL	1153	7.3			1/1
$k_{\text{ref}}: \text{CH}_3\text{CH}_3 \rightarrow \text{products}.$						
79 KAL/NAM ²⁾	RL	1153	1.29			1/1
$k_{\text{ref}}: \text{CH}_3(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{products}.$						
²⁾ Pyrolysis of hydrocarbon mixtures in a tubular reactor. Calculated rate ratios.						

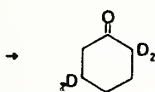
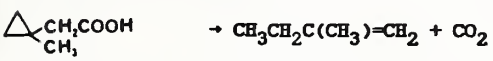
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k(k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
80 RUM/SHE Pyrolysis in a quartz reactor. P = 760 torr.	EX	883-993	3.31(13)	0	30216±1311	1	3.89
$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{products}$							
Pentane, 2-methyl-							
73 ILL/WEL P = 760 torr.	EX	853-1053	(1.03±0.03)(14)	0	29909	1	
$(\text{CH}_3)_3\text{CCH}_2\text{CH}_3 \rightarrow \text{products}$							
Butane, 2,2-dimethyl-							
73 ILL/WEL P = 760 torr.	EX	898-1053	(4.57±0.07)(13)	0	30191	1	
82 BIL/BAR Pyrolysis of 2,2-Dimethylbutane in a Pyrex vessel. Gas-chromatography. P = (50-150) torr.	EX	703-743	≈1.0(11)	0	25767	1	
$(\text{CH}_3)_3\text{CCH}_2\text{CH}_3 \xrightarrow{\dagger} \text{CH}_3 + (\text{CH}_3)_3\text{CCH}_2 \quad (\text{a})$							
$\rightarrow \text{CH}_3 + (\text{CH}_3)_2\text{CCH}_2\text{CH}_2 \quad (\text{b})$							
$\rightarrow \text{CH}_3\text{CH}_2 + (\text{CH}_3)_3\text{C} \quad (\text{c})$							
Butane, 2,2-dimethyl-							
72 HAS/JOH ¹⁾ $k_a + k_b + k_c$. P = 0.017 torr.	EX	298	(4.6±0.8)(5)			1	
72 HAS/JOH ¹⁾ $k_a + k_b + k_c$. P = 0.033 torr.	EX	298	(8.7±1.2)(5)			1	
¹⁾ $(\text{CH}_3)_3\text{CCH}_2\text{CH}_3 \xrightarrow{\dagger}$ formed by $^1\text{CH}_2 + (\text{CH}_3)_4\text{C}$.							
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CH} \quad (\text{a})$							
$\rightarrow \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{CHCHCH}_3 \quad (\text{b})$							
Butane, 2,3-dimethyl-							
74 GOL/ALF k_a . Best fit to experimental data to logA = 16.4 for each C-C fission.	DE	990-1250	2.51(16)	0	37544	1	
75 BUL/MAR k_a . Static system pyrolysis.	ES	667-770	1.58(16)	0	37649	1	
78 TSA4 ¹⁾	EX	990-1100	1.58(16)	0	38100	1	
78 TSA4 ¹⁾ Extrapolation over the given T-range.	EX	300-1100	1.82(17)	0	40800	1	
¹⁾ k_a . Single-pulse shock-tube.							
75 BUL/MAR k_b . Static system pyrolysis.	ES	667-770	1.0(17)	0	40416	1	
75 BUL/MAR $k_a + k_b$. Static system pyrolysis.	ES	667-770	5.01(16)	0	38732	1	

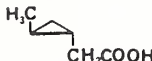
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{C}(\text{CH}_3)_2\text{COOH} \rightarrow \text{CH}_2=\text{C}(\text{CH}_3)_2 + \text{CO}_2$							
3-Butynoic acid, 2,2-dimethyl-							
76 BIG/WEA1	EX	500	2.44(-5)			1	
76 BIG/WEA1	EX	500-630	1.79(11)	0	18266±758	1	
A and B recalculated from the reported data.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{C}\equiv\text{CH} \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHC}\equiv\text{CH}$							
3-Butyn-1-ol acetate							
79 HER/CHU	EX	613-658	1.352(13)	0	23732±192	1	1.35
Pyrolysis in a static system. P = (53-180) torr.							
$(\text{CH}_2=\text{CHCH}_2)_2\text{O} \rightarrow \text{CH}_2=\text{CHCHO} + \text{CH}_3\text{CH}=\text{CH}_2$							
1-Propene, 3,3'-oxybis- (Diallylether)							
→ 2-Propenal (Acrolein) + 1-Propene							
74 VII/EGG3	EX	545-627	6.76(11)	0	20584±176	1	1.35
Pyrolysis in a static system. P = (4-84) torr.							
 →  (a) →  (b) → other products (c)							
7-Oxabicyclo[4.1.0]heptane (1,2-Epoxy-cyclohexane)							
→ 2-Cyclohexen-1-ol (a)							
→ Cyclohexanone (b)							
→ other products (c)							
73 FLO/PEN1 ¹⁾	EX	680-740	1.29(13)	0	28082±654	1	2.57
k_a . P = (1.6-6) torr.							
74 FLO/PEN2 ¹⁾	EX	677-746	1.86(13)	0	28420±755	1	2.88
k_a . P = 4 torr.							
73 FLO/PEN1 ¹⁾	EX	680-740	3.80(14)	0	30347±554	1	2.24
k_b . P = (1.6-6) torr.							
74 FLO/PEN2 ¹⁾	EX	677-746	6.31(14)	0	30820±710	1	2.69
k_b . P = 4 torr.							
73 FLO/PEN1 ¹⁾	EX	677-736	1.38(14)	0	29190±554	1	2.19
$k_a + k_b + k_c$.							
P = (1.6-6) torr.							
74 FLO/PEN2 ¹⁾	EX	677-746	2.29(14)	0	29653±846	1	3.31
$k_a + k_b + k_c$.							
P = 4 torr.							
¹⁾ Thermolysis in a static system.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
  other products (c)							
7-Oxabicyclo[4.1.0]heptane-2,2,5,5-d ₄ (1,2-Epoxycyclohexane-2,2,5,5-d ₄)							
→ 2-Cyclohexen-3,6,6-d ₃ -ol-d (a)							
→ Cyclohexanone-2,2,5,5-d ₄ (b)							
→ other products (c)							
74 FLO/FEN2 ¹⁾ k _a . P = 4 torr.	EX	677-746	2.19(13)	0	29225±493	1	2.0
74 FLO/FEN2 ¹⁾ k _b . P = 4 torr.	EX	677-746	7.24(14)	0	30951±523	1	2.09
74 FLO/FEN2 ¹⁾ k _a + k _b + k _c . P = 4 torr.	EX	677-746	4.47(14)	0	30398±760	1	2.88
¹⁾ Thermolysis in a static system.							
CH ₂ =CHC(CH ₃) ₂ COOH → CH ₂ =CHCH(CH ₃) ₂ + CO ₂ 3-Butenoic acid, 2,2-dimethyl-							
82 ALB/BIG ¹⁾	EX	577	9.7(-4)				1
82 ALB/BIG ¹⁾	EX	~577	1.03(11)	0	18619		1
A and B recalculated from the reported data.							
¹⁾ Pyrolysis in a flow-reactor. NMR-spectrometry.							
CH ₃ C(O)OCH ₂ CH ₂ CH=CH ₂ → CH ₃ COOH + CH ₂ =CHCH=CH ₂ 3-Buten-1-ol acetate							
79 MAR/HER	EX	513-693	1.58(13)	0	24153±253	1	1.48
Pyrolysis in a static system. Gas-chromatography. P = (44-282) torr.							
 Cyclopropaneacetic acid, 1-methyl- → 1-Propene, 2-methyl- + Carbon dioxide							
79 BIG/FET ¹⁾	EX	725	(8.24±0.35)(-2)				1
79 BIG/FET ¹⁾	EX	690-740	(4.62±0.20)(11)	0	21282±1311		1
A and B recalculated from the reported data.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
1) Pyrolysis in a Flow-reactor with evacuated sealed tubes. Gas-chromatography. NMR-spectroscopy.  $\rightarrow (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 + \text{CO}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 + \text{CO}_2$ (b) $\rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CO}_2$ (c) Cyclopropaneacetic acid, 2-methyl-, trans- $\rightarrow$ 1-Butene, 3-methyl- + Carbon dioxide (a) $\rightarrow$ 1-Pentene + Carbon dioxide (b) $\rightarrow$ 1-Butene, 2-methyl- + Carbon dioxide (c)							
80 BIG/FET ¹⁾ k _a .	EX	725	1.13(-3)				1
80 BIG/FET ¹⁾ k _b .	EX	725	5.7(-4)				1
80 BIG/FET ¹⁾ k _c . Upper-limit k.	EX	725	<4.0(-5)				1
80 BIG/FET ¹⁾ k _a + k _b + k _c .	EX	725	1.7(-3)				1
80 BIG/FET ¹⁾ k _a + k _b + k _c . A and B recalculated from the reported data.	EX	750-820	3.31(11)	0	23855±601		1
1) Pyrolysis in a flow-reactor with evacuated sealed tubes. Gas-chromatography. NMR-spectrometry. $\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_3\text{C}(\text{O})\text{CH}=\text{CH}_2$ 2-Butanone, 4-(acetyloxy)-							
72 TIN/KOO Thermolysis.	EX	587-636	7.94(12)	0	18520±503	1	2.51
$(\text{CH}_3)_2\text{CHCH}_2\text{OCH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3\text{CHO}$ Propane, 1-(ethenyloxy)-2-methyl-							
74 BAM Thermolysis in a static system. Gas-chromatography.	EX	653-708	3.80(10)	0	20990±120	1	1.20
$(\text{CH}_3)_2\text{CHOC}(\text{CH}_3)=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CO} + \text{CH}_3\text{CH}=\text{CH}_2$ 1-Propene, 2-(1-methylethoxy)-							
81 FLO/HON Thermolysis in a static system.	EX	554-613	9.55(11)	0	20220±613	1	2.88

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$(\text{CH}_3)_3\text{COCH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CHO} + (\text{CH}_3)_2\text{C}=\text{CH}_2$							
Propane, 2-(ethenyloxy)-2-methyl-							
79 ROS/GOL	EX	625-925	1.0(12)	0	19326±503	1	1.86
VLP-Pyrolysis.							
High-pressure k.							
RRKM best data-fit.							
$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{CH}_2\text{C}-\text{C}-\text{CH}_3 \\ \\ \text{CH}_3 \end{array} \rightarrow \text{HCHO} + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$							
Oxetane, 3-ethyl-3-methyl-							
75 CLE/FRE	EX	680-721	2.28(15)	0	30219±243	1	1.42
Thermolysis in a static system.							
$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C}-\text{C}-\text{CH}_3 \\ \quad \\ \text{H}_3\text{C} \quad \text{CH}_3 \end{array} \rightarrow \begin{array}{ll} \text{CH}_3\text{COC}(\text{CH}_3)_3 & \text{(a)} \\ \text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)_2\text{OH} & \text{(b)} \\ \text{CH}_3\text{CH}=\text{CH}_2 + (\text{CH}_3)_2\text{CO} & \text{(c)} \end{array}$							
Oxirane, tetramethyl-							
→ 2-Butanone, 3,3-dimethyl- (a)							
→ 1-Buten-3-ol, 2,3-dimethyl- (b)							
→ 1-Propene + 2-Propanone (c)							
81 FLO/HON ¹⁾	EX	642-733	3.72(13)	0	28074±746	1	2.88
k _a .							
81 FLO/HON ¹⁾	EX	642-733	6.46(11)	0	25236±1504	1	8.71
k _b .							
81 FLO/HON ¹⁾	EX	642-733	3.55(13)	0	28267±541	1	2.19
k _c .							
¹⁾ Thermolysis in a static system.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2$							
Acetic acid butyl ester (n-Butyl acetate)							
72 TIN/KOO	EX	668-741	2.51(12)	0	23805±252	1	1.58
Thermolysis.							
76 DEB/TAY	EX	650-700	3.98(12)	0	24207	1	
$\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}_2\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$							
Propanoic acid 1-methylethyl ester							
77 CHU/MAR	EX	563-623	1.15(13)	0	22849±101	1	1.23
77 SMI/MUT	EX	651	(6.10±0.20)(-3)			1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{COOH} + (\text{CH}_3)_2\text{C}=\text{CH}_2$							
Acetic acid 1,1-dimethylethyl ester (t-Butyl acetate)							
75 TAY ¹⁾	EX	557-609	2.0(13)	0	20282±176	1	1.26
78 AMI/TAY1 ¹⁾	EX	518-609	1.15(13)	0	199975	1	
¹⁾ Pyrolysis in a stainless-steel reactor.							
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CD}_3)_3 \rightarrow \text{CH}_3\text{COOD} + (\text{CD}_3)_2\text{C}=\text{CD}_2$							
Acetic acid 1,1-dimethylethyl-d ₉ ester (t-Butyl-d ₉ acetate)							
78 AMI/TAY1	EX	558-608	2.4(13)	0	20921	1	
Pyrolysis in a stainless-steel reactor.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{OCH}_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{OCH}_3$							
1-Propanol, 3-methoxy-, acetate							
76 DEB/TAY	EX	650-700	4.47(12)	0	24409	1	
$\text{CH}_3\text{OCH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{OCH}_2\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$							
Acetic acid, methoxy-, 1-methylethyl ester							
77 SMI/MUT	EX	651	(6.87±0.27)(-3)			1	
78 CHU/MAR ¹⁾	EX	603	5.89(-4)			1	
78 CHU/MAR ¹⁾	EX	583-633	1.10(13)	0	22597±151	1	1.35
¹⁾ Pyrolysis in a static system.							
$\text{CH}_3\text{CH}_2\text{OC}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_3$							
$\rightarrow \text{CH}_2=\text{CH}_2 + \text{CO}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$ (a)							
$\rightarrow \text{CH}_3\text{CH}_2\text{OH} + \text{CO}_2 + \text{CH}_3\text{CH}=\text{CH}_2$ (b)							
Carbonic acid ethyl propyl ester (Ethyl propyl carbonate)							
76 CRO/HUN	EX	581-664	7.76(11)	0	21843	1	
$k_a + k_b$.							
$(\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CO}$ (a)							
$\rightarrow (\text{CH}_3)_2\text{CHCOCH}_3 + \text{CH}_3$ (b)							
Propoxy, 1,1,2-trimethyl-							
75 ALC/MIL	ES	373	4.7(6)			1	
k_a .							
75 ALC/MIL	ES	373	1.5(8)			1	
k_b .							
$(\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2 + \text{O}_2 \rightarrow \text{products}$							
Propoxy, 1,1,2-trimethyl- + Oxygen molecule							
75 ALC/MIL	ES	373	1.2(9)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$ $\rightarrow (\text{CH}_3)_2\text{CHCH}(\text{OH})(\text{CH}_3)_2 + (\text{CH}_3)_2\text{CHC}(\text{CH}_3)_2$ Propoxy, 1,1,2-trimethyl- + Butane, 2,3-dimethyl- 75 ALC/MIL	ES	373	4.0(8)			2
$(\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$ $\rightarrow (\text{CH}_3)_2\text{CHC}(\text{OOH})(\text{CH}_3)_2 + (\text{CH}_3)_2\text{CHC}(\text{CH}_3)_2$ Propyldioxy, 1,1,2-trimethyl- + Butane, 2,3-dimethyl- 75 ALC/MIL	ES	373	1.6(5)			2
$(\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2 + (\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2$ $\rightarrow (\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2$ $+ (\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2 + \text{O}_2$ (a) $\rightarrow$ Fragmentation products (b) Propyldioxy, 1,1,2-trimethyl- 75 ALC/MIL k_a .	ES	373	2.3(11)			2
75 ALC/MIL k_b .	ES	373	2.4(11)			2
$(\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CHC}(\text{O})\text{CH}_3 + \text{CH}_3$ (a) $\rightarrow (\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CO}$ (b) Propyldioxy, 1,1,2-trimethyl- 77 ALC/MIL ¹⁾	RN	373	1.5(8)			1
k_a . (α -scission). Estimated k. 77 ALC/MIL ¹⁾	RN	373	4.7(6)			1
k_b . (β -scission). Estimated k. ¹⁾ Azomethane photolysis.						
$(\text{CH}_3)_2\text{CHC}(\text{CH}_3)_2\text{OH} \rightarrow (\text{CH}_3)_2\text{CH} + \text{C}(\text{CH}_3)_2\text{OH}$ (a) $\rightarrow (\text{CH}_3)_2\text{CHC}(\text{CH}_3)=\text{CH}_2 + \text{H}_2\text{O}$ (b) $\rightarrow (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{H}_2\text{O}$ (c) 2-Butanol, 2,3-dimethyl- 76 TSA1	EX	1080-1165	1.74(16)	0	37400	1
k_a . 76 TSA1	EX	1080-1165	1.48(14)	0	32300	1
k_b . 76 TSA1	EX	1080-1165	4.57(13)	0	32700	1
k_c .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_3\text{CCH}(\text{CH}_3)\text{OH} \rightarrow (\text{CH}_3)_3\text{C} + \text{CH}_3\text{CHOH} \quad (\text{a})$ $\rightarrow (\text{CH}_3)_3\text{CCH}=\text{CH}_2 + \text{H}_2\text{O} \quad (\text{b})$						
2-Butanol, 3,3-dimethyl-						
76 TSA1	EX	990-1125	2.14(16)	0	37500	1
k_a .						
76 TSA1	EX	990-1125	<1.0(14)	0	34200	1
k_b .						
Upper-limit k.						
$\text{CH}_2=\text{CHCH}_2\text{SCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHCHS} + \text{CH}_3\text{CH}=\text{CH}_2$						
1-Propene, 3,3'-thiobis- (Diallyl sulfide)						
$\rightarrow$ 2-Propenethial + 1-Propene						
82 MAR/ROP2	EX	588-691	1.02(11)	0	16960±84	1 1.15
Pyrolysis in a stirred-flow system.						
2-Propenethial (Thioacrolein) polymerizes into a film. Mass-spectrometry.						
P = (2-15) torr.						
$\text{CH}_3\text{CH}_2\text{CH}_2\text{SCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CHS} + \text{CH}_3\text{CH}=\text{CH}_2$						
1-Propene, 3-(propenylthio)-						
$\rightarrow$ Propanethial + 1-Propene						
82 MAR/ROP1 ¹⁾	EX	543-673	3.31(11)	0	18885±241	1 1.45
82 MAR/ROP1 ¹⁾	SE	535-680	1.15(11)	0	18355±352	1 1.15
Alternate expression, including the previous (static) and the present (flow) measurements.						
¹⁾ Pyrolysis in a static system. Mass- and NMR-spectrometry. Propanethial trimerizes into the cyclic compound: 2,4,6-Triethyl-1,3,5-trithiane.						
P(Total) =(2-18) torr.						
$\text{CH}_3\text{C}(\text{S})\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{COS} + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \quad (\text{a})$ $\rightarrow \text{CH}_3\text{C}(\text{O})\text{SCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \quad (\text{b})$						
Ethanethioic acid O-butyl ester						
75 BIG/GAB ¹⁾	EX	635	2.16(-2)			1
k_a . Elimination.						
75 BIG/GAB ¹⁾	EX	613-641	2.51(12)	0	20382	1
k_a . Elimination.						
75 BIG/GAB ¹⁾	EX	629	2.86(-3)			1
k_b . Isomerization.						
75 BIG/GAB ¹⁾	EX	613-641	7.94(11)	0	20886	1
k_b . Isomerization.						
75 BIG/GAB ¹⁾	EX	633	2.97(-2)			1
$k_a + k_b$. Overall reaction.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 BIG/GAB $k_a + k_b$. Overall reaction. 1) Flow-reactor pyrolysis.	EX	613-641	1.26(12)	0	19829	1
$\text{CH}_3\text{C}(\text{S})\text{OCH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ → $\text{CH}_4 + \text{COS} + \text{cis-CH}_3\text{CH=CHCH}_3$ (a) → $\text{CH}_4 + \text{COS} + \text{trans-CH}_3\text{CH=CHCH}_3$ (b) → $\text{CH}_4 + \text{COS} + \text{CH}_2=\text{CHCH}_2\text{CH}_3$ (c)						
Ethanethioic acid O-(1-methylpropyl) ester 75 BIG/GAB 1) 75 BIG/GAB 1) 75 BIG/GAB 1) 1) $k_a + k_b + k_c$. Elimination. Flow-reactor pyrolysis. Probably isomerization not occurring.	EX	571 629 545-575	3.4(-2) 7.33(-1) 2.51(12)			1 1 1
$\text{CH}_3\text{C}(\text{S})\text{OCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{COS} + (\text{CH}_3)_2\text{C=CH}_2$ (a) → $\text{CH}_3\text{C}(\text{O})\text{SH}_2\text{CH}(\text{CH}_3)_2$ (b)						
Ethanethioic acid O-(2-methylpropyl) ester 75 BIG/GAB 1) k_a . Elimination. 75 BIG/GAB 1) k_a . Elimination. 75 BIG/GAB 1) k_b . Isomerization. 75 BIG/GAB 1) $k_a + k_b$. Overall reaction. 75 BIG/GAB 1) $k_a + k_b$. Overall reaction. 1) Flow-reactor pyrolysis.	EX	629 623-657 629 649 623-657	1.30(-2) 3.55(12) 2.49(-3) 4.38(-2) 1.58(12)			1 1 1 1 1
$\text{CH}_3\text{C}(\text{O})\text{SCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{COS} + \text{CH}_2=\text{CHCH}_2\text{CH}_3$ Ethanethioic acid S-butyl ester 73 BIG/GAB 1) 73 BIG/GAB 1) 1) Elimination. Flow-reactor pyrolysis.	EX	790 780-810	3.0(-2) 3.98(11)			1 1
$\text{CH}_3\text{C}(\text{O})\text{SCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{COS} + (\text{CH}_3)_2\text{C=CH}_2$ Ethanethioic acid S-(2-methylpropyl) ester 73 BIG/GAB 1) 73 BIG/GAB 1) 1) Elimination. Flow-reactor pyrolysis.	EX	804 790-825	3.3(-2) 6.31(11)			1 1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k. err. units factor
CH₃C(O)SCH(CH₃)CH₂CH₃						
→ CH ₄ + COS + cis-CH ₃ CH=CHCH ₃ (a)						
→ CH ₄ + COS + trans-CH ₃ CH=CHCH ₃ (b)						
→ CH ₄ + COS + CH ₂ =CHCH ₂ CH ₃ (c)						
Ethanethioic acid S-(1-methylpropyl) ester						
73 BIG/GAB ¹⁾	EX	730	3.2(-2)			1
73 BIG/GAB ¹⁾	EX	714-743	5.01(11)	0	22144±604	1
¹⁾ k _a + k _b + k _c . Elimination. Flow-reactor pyrolysis.						
CH₃C(O)SC(CH₃)₃ → CH₄ + COS + (CH₃)₂C=CH₂						
Ethanethioic acid S-(1,1-dimethylethyl) ester						
72 OEL/TIN	EX	653-705	6.31(13)	0	23000	1
Elimination by thermolysis.						
73 BIG/GAB ¹⁾	EX	652	1.8(-2)			1
73 BIG/GAB ¹⁾	EX	650-680	1.58(12)	0	20936±201	1
¹⁾ Elimination. Flow-reactor pyrolysis.						
CH₃OC(O)SC(CH₃)₃ → CH₃OH + C(O)S + CH₂=C(CH₃)₂						
Carbonothioic acid S-(1,1-dimethylethyl)						
O-methyl ester						
79 ALA/BIG ¹⁾	EX	629	1.2(-3)			1
79 ALA/BIG ¹⁾	EX	643-693	1.35(12)	0	21799±722	1
A and B recalculated from the reported data. ¹⁾ Flow-reactor pyrolysis. (Flow-tube method.)						
(CH₃)₃COC(O)SCH₃ → (CH₃)₂C=CH₂ + CO₂ + CH₃SH						
Carbonothioic acid O-(1,1-dimethylethyl)						
S-methyl ester						
79 ALA/BIG ¹⁾	EX	629	4.2(-4)			1
79 ALA/BIG ¹⁾	EX	752-775	4.88(10)	0	16025±203	1
A and B recalculated from the reported data. ¹⁾ Flow-reactor pyrolysis. (Inhibited tube method.)						
CH₃C(S)SCH₂CH₂CH₂CH₃ → CH₄ + CS₂ + CH₂=CHCH₂CH₃						
Ethane(dithioic) acid butyl ester						
78 ALA/BIG ¹⁾	EX	629	3.3(-3)			1
78 ALA/BIG ¹⁾	EX	651-716	1.08(13)	0	22473	1
A and B recalculated from the reported data. ¹⁾ Flow-reactor pyrolysis.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{C}(\text{S})\text{SCH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{cis-CH}_3\text{CH=CHCH}_3$ (a)						
$\rightarrow \text{trans-CH}_3\text{CH=CHCH}_3$ (b)						
$\rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}_3$ (c)						
Ethane(dithioic) acid 1-methylpropyl ester						
78 ALA/BIG ¹⁾	EX	629	7.4(-2)			1
78 ALA/BIG ¹⁾	EX	584-639	6.67(12)	0	22211	1
A and B recalculated from the reported data.						
¹⁾ $k_a + k_b + k_c$.						
Pyrolysis in a flow-reactor.						
$\text{CH}_3\text{C}(\text{S})\text{SC}(\text{CH}_3)_3 \rightarrow \text{CH}_4 + \text{CS}_2 + \text{CH}_2=\text{C}(\text{CH}_3)_2$						
Ethane(dithioic) acid 1,1-dimethylethyl ester						
78 ALA/BIG ¹⁾	EX	629	3.1(-1)			1
78 ALA/BIG ¹⁾	EX	448-502	1.05(13)	0	19598	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a flow-reactor.						
$\text{CH}_3\text{OC}(\text{S})\text{SC}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{OH} + \text{CS}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2$						
Carbonodithioic acid S-(1,1-dimethylethyl) O-methyl ester						
82 ALA/BIG ¹⁾	EX	629	4.3(-1)			1
82 ALA/BIG ¹⁾	EX	540-570	1.90(11)	0	16867	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a flow reactor.						
IR-spectrometry.						
P = (2-800) torr.						
 $\rightarrow \text{CH}_2=\text{CHCN} + \text{CH}_2=\text{CHCN}$						
1,2-Cyclobutanedicarbonitrile, trans-						
72 SAR/GAL	EX	726-783	2.51(12)	0	20735	1
Thermolysis in a flow-reactor.						
Gas-chromatography.						
 $\rightarrow \text{CH}_2=\text{C}=\text{CH}_2 + \text{CH}_2=\text{CHCN}$						
1-Cyclobutanecarbonitrile, 3-methylene-						
72 SAR/GAL ¹⁾	EX	726-783	5.01(12)	0	24711	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
72 SAR/GAL ¹⁾ Average between the previous and present data.	SE	726-783	5.27(12)	0	24711	1
¹⁾ Thermal isomerization in a flow-reactor. Gas-chromatography.						
Cyclopropanamine, N-propylidene- → 2H-Pyrrole, 2-ethyl-3,4-dihydro- (5-Ethyl-1-pyrroline)						
72 COC/EGG1 Thermolysis in a static system. Gas-chromatography. P-independent k from 2.5 to 55 torr.	EX	573-635	1.12(14)	0	24041±81	1 1.15
2H-Pyrrole, 2-ethyl-3,4-dehydro- (5-Ethyl-1-pyrroline) → 3H-Pyrrole, 2-ethyl- + Hydrogen molecule						
72 COC/EGG2 Pyrolysis in a static system. Gas-chromatography. P = (12-60) torr.	EX	721-786	3.16(12)	0	27932±700	1 2.51
$\text{CH}_2=\text{CHCH}_2\text{NCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_2=\text{CHCH}=\text{NH}$						
2-Propen-1-amine, N-(2-propenyl)- 74 EGG/VIT1	EX	533-616	1.10(11)	0	18676±166	1 1.35
$(\text{CH}_3)_2\text{CHN}=\text{NCH}_2\text{CH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CH} + \text{CH}_2\text{CH}=\text{CH}_2 + \text{N}_2$						
Diazene, (1-methylethyl)-2-propenyl- 72 CRA/TAK Thermolysis. Gas-chromatography. Mass-spectrometry. In presence of ¹⁵ NO. P(Total) = (50-60) torr.	EX	374-399	6.31(14)	0	17916±252	1 1.91

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{CH}_2\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_2\text{CH}_3^* \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2 + \text{N}_2$							
Diazene, dipropyl- (Azo-n-propane)							
77 CHE/ORE Azo-n-propane/He high-pressure photolysis. RRKM data-fit on the basis of a proposed mechanism. Azo-n-propane assumed to be in vibrationally excited T_1 electronic state. Lower-limit k. $P(\text{CO}_2) = (0-45)$ atm. $P(\text{He}) = (0-50)$ atm.	EX	298	4.0(7)			1	
81 ADA/BAS1 Flash-photolysis in N_2 . Kinetic spectroscopy.	EX	298	(6.6±1.3)(7)			1	
$(\text{CH}_3)_2\text{CHN}=\text{NCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CH} + \text{N}_2$							
Diazene, bis(1-methylethyl)- (Azoisopropane)							
73 PER/BEA RRKM fit of experimental data.	EX	625-830	3.98(16)	0	24107±503	1	
77 MCK/TUR ¹⁾ Series A Pyrolysis.	EX	503-544	2.04(16)	0	23956±849	1	4.90
77 MCK/TUR ¹⁾ Series B Pyrolysis.	EX	518-573	2.14(17)	0	25437±309	1	1.74
¹⁾ Static system thermolysis.							
79 SZI Static system thermolysis.	EX	494-446	3.98(14)	0	21411±481	1	2.51
80 ACS/PET Thermolysis in a high-vacuum system.	EX	523-623	1.58(16)	0	23672±313	1	2.0
82 MCM/LEW ²⁾ Experimental rate expression.	EX	780-1025	3.24(13)	0	19930±503	1	1.12
82 MCM/LEW ²⁾ Best fit to present and previous data.	SE	780-1025	7.94(13)	0	20735	1	
²⁾ Laser-powered homogeneous pyrolysis in excess Toluene, or Cumene as scavengers.							
$(\text{CH}_3)_2\text{CHN}=\text{NCH}(\text{CH}_3)_2^* \rightarrow (\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CH} + \text{N}_2$							
Diazene, bis(1-methylethyl)- (Azoisopropane)							
77 CHE/ORE Azoisopropane/He high-pressure photolysis. RRKM data-fit on the basis of a proposed mechanism. Azoisopropane is assumed to be be in a vibrationally excited T_1 electronic state. Lower-limit k. $P(\text{CO}_2) = (0-45)$ atm. $P(\text{He}) = (0-100)$ atm.	EX	298	5.0(8)			1	
81 ADA/BAS1 Flash-photolysis in N_2 . Kinetic spectroscopy.	EX	298	(1.6±0.4)(8)			1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{CONEC}(\text{CH}_3)_3 (+ \text{M}) \rightarrow \text{CH}_3\text{CONH}_2 + (\text{CH}_3)_2=\text{CH}_2 (+ \text{M})$ (a)							
$\rightarrow \text{CH}_2=\text{C}=\text{O} + (\text{CH}_3)_3\text{CNH}_2 (+ \text{M})$ (b)							
Acetamide, N-(1,1-dimethylethyl)-							
$\rightarrow$ Acetamide + 1-Propene, 2-methyl- (a)							
$\rightarrow$ Ethenone + 2-Propanamine, 2-methyl- (b)							
73 MAC/NAG ¹⁾	EX	658-738	2.63(12)	0	25939±533	1	2.14
k_a . Six-centered transition state assumed.							
73 MAC/NAG ¹⁾	EX	673-725	3.63(13)	0	17589±644	2	2.51
k_b . M = CH ₃ COOH.							
¹⁾ Vacuum-system pyrolysis.							
P-independent k within the given P-range.							
Acetic acid catalysis.							
P = (52-412) torr.							
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{CN} \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{C}(\text{CH}_3)\text{CN}$							
Propanenitrile, 2-(acetyloxy)-2-methyl-							
80 MAR/CHU	EX	503-613	2.82(14)	0	23901±1059	1	6.61
Static system pyrolysis. Mass-spectrometry.							
IR-, and NMR-spectroscopy.							
P = (56-210) torr.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{N}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHN}(\text{CH}_3)_2$							
Acetic acid 2-(dimethylamino)ethyl ester							
80 CHU/MAR	EX	592-723	7.94(13)	0	6511±457	1	2.0
Pyrolysis in a static system.							
Gas-chromatography.							
P = (63-207) torr.							
$(\text{CH}_3)_2\text{NC}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{NH} + \text{CO}_2 + \text{CH}_3\text{CH}=\text{CH}_2$							
Carbamic acid, dimethyl-, 1-methylethyl ester							
72 DAL/ZIO2	EX	323-333	1.10(13)	0	21797±201	1	
Pyrolysis in a conventional static system.							
$\text{CH}=\text{CCH}_2\text{CH}_2\text{CH}_2\text{C}=\text{CH} \rightarrow \text{CH}_2=\text{C}=\text{CH}_2 + \text{CH}_2=\text{CHC}=\text{CH}$							
1,6-Heptadiyne							
80 KIN	EX	794-1225	3.98(12)	0	26019±503	1	2.51
VLP-Pyrolysis.							
High-pressure k extrapolated from							
VLPP data by means of RRKM theory.							
$\text{CH}_2=\text{C}=\text{CHCH}(\text{CH}_3)\text{C}=\text{CH} \rightarrow \text{CH}=\text{CCH}_2\text{CH}=\text{C}=\text{CHCH}_3$							
1,2-Hexadien-5-yne, 4-methyl-							
72 HOP	EX	423-473	6.92(10)	0	15501±151	1	1.35

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 $\rightarrow$ 							
1,3,5-Cycloheptatriene $\rightarrow$ Benzene, methyl- (Toluene)							
75 LUU/GLA ¹⁾	EX	900-1300	3.16(13)	0	25140 $\pm$ 722	1	1.58
75 LUU/GLA ¹⁾	SE	600-1300	6.31(13)	0	26222 $\pm$ 120	1	1.12
Extended Arrhenius expression over the low and high T-range, by combining the previous and the present data.							
¹⁾ M = Ar. Thermal isomerization behind incident and reflected shock-waves. Total Conc. = (0.6-6.0) $\times 10^{18}$ molec.cm ⁻³ . [Cycloheptatriene] = (0.01-1.0)% P-independent k.							
 $\rightarrow$  $+ \text{CH}\equiv\text{CH}$ (a)							
$\rightarrow$  (b)							
$\rightarrow$  (c)							
Bicyclo[2.2.1]hepta-2,5-diene (2,5-Norbornadiene) $\rightarrow$ 1,3-Cyclopentadiene + Ethyne (a) $\rightarrow$ 1,3,5-Cycloheptatriene (b) $\rightarrow$ Benzene, methyl- (Toluene) (c)							
75 WAL/WEL ¹⁾	EX	584-630	6.03(14)	0	25853 $\pm$ 146	1	1.26
k _a . Decomposition.							
75 WAL/WEL ¹⁾	EX	584-630	7.94(14)	0	25848 $\pm$ 151	1	1.29
k _b + k _c . Isomerization by ring expansion and by rearrangement.							
¹⁾ Decomposition in a static vacuum system.							
 $\rightarrow$  $+ \text{CH}_2=\text{CH}_2$							
Bicyclo[2.2.1]hept-2-ene (Norbornene) $\rightarrow$ 1,3-Cyclopentadiene + Ethene							
76 WAL/WEL	EX	521-570	1.8(14)	0	22420 $\pm$ 360	1	1.9
Decomposition of Norbornene in a static system.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
  (a)  + CH ₂ =CH ₂ (b) → cis-CH ₂ =CHCH=CHCH=CHCH ₃ → products (c)							
Bicyclo[3.2.0]hept-2-ene							
→ -Bicyclo[2.2.1]hept-2-ene (Norbornene) (a)							
→ 1,3-Cyclopentadiene + Ethene (b)							
→ 1,3,6-Heptatriene, (Z)- → products (c)							
71 COC/FRE2 ¹⁾ k _a . Isomerization.	ES	580-626	2.24(11)	0	21062±528	1	2.40
71 COC/FRE2 ¹⁾ k _b . Decomposition.	ES	580-626	7.94(15)	0	26850±453	1	2.14
71 COC/FRE2 ¹⁾ k _{overall} . Isomerization by decyclization.	ES	580-626	3.16(12)	0	23150±1812	1	2.0
The products formed by further isomerization are believed to be:							
1-Methyl-1,3-Cyclohexadiene,							
2-Methyl-1,3-Cyclohexadiene,							
5-Methyl-1,3-Cyclohexadiene,							
1,3,5-Heptatriene, (E,E)- (trans,trans)							
1,3,5-Heptatriene, (Z,Z)- (cis,cis).							
71 COC/FRE2 ¹⁾ k _a + k _b .	EX	580-626	7.08(14)	0	25174±302	1	1.62
71 COC/FRE2 ¹⁾ k _{overall} .	EX	580-626	5.75(14)	0	24979±121	1	1.23
¹⁾ Pyrolysis in a conventional static system. Gas-chromatography. The k's for the channels (a), (b) and (c), subject to errors, are given with caution. P = torr.							
 → CH ₂ =C=CHCH ₂ CH ₂ CH=CH ₂ (a) → CH ₂ =CHC(=CH ₂)CH ₂ CH=CH ₂ (b)							
Tricyclo[4.1.0.0 ^{1,3}]heptane							
→ 1,2,6-Heptatriene (a)							
→ 1,5-Hexadiene, 3-methylene- (b)							
71 FRE/HOP ¹⁾ k _a .	EX	423-463	1.2(14)	0	18740±332	1	2.14

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
71 FRE/HOP ¹⁾ k_b . ¹⁾ Thermal isomerization in a static system. k is P-independent within the (0.2-2.3) torr. range. Gas-chromatography.	EX	423-463	1.62(14)	0	17898±126	1	1.32
$\text{CH}\equiv\text{CCH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}\equiv\text{CCH}_2 + \text{CH}_3\text{CHCH}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_2=\text{C}=\text{CH}_2 + \text{CH}_2=\text{CHCH}_2\text{CH}_3$ (b)							
1-Hexyne, 4-methyl-							
78 TSA3 ¹⁾ k_a . Bond-breaking reaction.	EX	990-1200	7.94(15)	0	35000±500	1	1.58
78 TSA3 ¹⁾ k_b . Molecular reaction.	EX	990-1200	7.94(12)	0	28000±1000	1	2.51
¹⁾ 4-Methyl-1-hexyne/Cyclohexene/Toluene/Ar thermolysis in a single-pulse shock-tube. k's determined relative to the decomposition of Cyclohexane. Similar data given 76 TSA2. [4-Methyl-1-hexyne] = 0.02%. [Cyclohexene] = 0.01%. P(Ar) ~ (2-6) atm. [Toluene] = 1%.							
$\text{CH}\equiv\text{CCH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}\equiv\text{CCH}_2 + \text{CH}_2\text{CH}(\text{CH}_3)_2$ (a) $\rightarrow \text{CH}_2=\text{C}=\text{CH}_2 + \text{CH}_2=\text{C}(\text{CH}_3)_2$ (b)							
1-Hexyne, 5-methyl-							
78 TSA3 ¹⁾ k_a . Bond-breaking reaction.	EX	990-1200	1.26(16)	0	36700±500	1	1.58
78 TSA3 ¹⁾ k_b . Molecular reaction.	EX	990-1200	2.00(12)	0	27500±1000	1	2.51
¹⁾ 5-Methyl-1-hexyne/Cyclohexene/Toluene/Ar thermolysis in a single-pulse shock-tube. k's determined relative to the decomposition of Cyclohexane. Similar data given in 76 TSA2. [5-Methyl-1-hexyne] = 0.02%. [Cyclohexene] = 0.01%. P(Ar) ~ (2-6) atm. [Toluene] = 1%.							
$\text{CH}_3\text{C}\equiv\text{C}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{C}\equiv\text{C}(\text{CH}_3)_2 + \text{CH}_3$							
2-Pentyne, 4,4-dimethyl-							
81 KIN/NGU Thermolysis in a VLPP system. Mass-spectrometry.	EX	903-1246	2.51(16)	0	35934±755	1	2.0

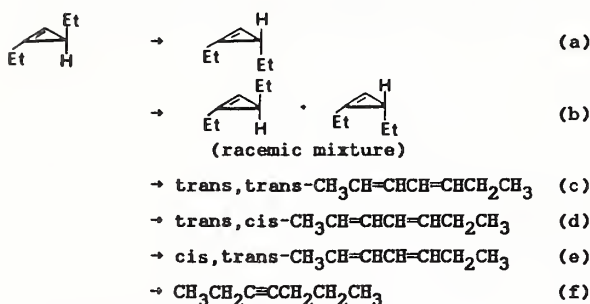
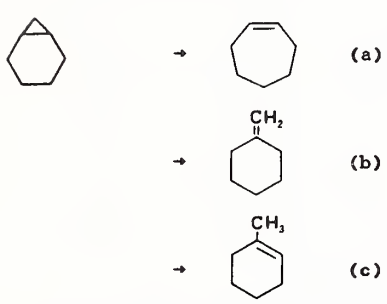
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2$							
1,6-Heptadiene							
74 EGG/VIT3 Thermolysis in a static system.	EX	628-744	2.04(11)	0	23654±367	1	2.75
80 KIN VLP-Pyrolysis. RRKM extrapolation of VLPP data.	EX	794-1225	2.00(11)	0	23704±503	1	2.51
$\text{cis-CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CHCH}_3$ → $\text{trans-CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CHCH}_3$ (a) → $\text{CH}_2=\text{CHC}(\text{CH}_3)=\text{C}(\text{CH}_3)_2$ (b)							
1,3-Pentadiene, 2,3-dimethyl- (Z)- → 1,3-Pentadiene, 2,3-dimethyl-, (E)- (a) → 1,3-Pentadiene, 3,4-dimethyl- (b)							
71 FRE/LAM ¹⁾ k _a .	RN	473-517	1.78(12)	0	22096±192	1	1.35
71 FRE/LAM ¹⁾ k _b .	DE	473-517	9.33(10)	0	16732±108	1	1.26
¹⁾ Thermal isomerization in static system. Gas-chromatography. k is P-independent between 0.75 and 7.5 torr. k's determined from Equilibrium constants and the sums (k _a + k _{-a}) and (k _b + k _{-b}).							
$\text{trans-CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CHCH}_3$ → $\text{cis-CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CHCH}_3$							
1,3-Pentadiene, 2,3-dimethyl-, (E)- → 1,3-Pentadiene, 2,3-dimethyl-, (Z)-							
71 FRE/LAM Thermal isomerization in a static system. Gas-chromatography. k is P-independent between 0.75 and 7.5 torr. k determined from Equilibrium constant and the sum (k _f + k _r).	DE	473-517	2.29(12)	0	22770±192	1	1.35
$\text{CH}_2=\text{CHC}(\text{CH}_3)=\text{C}(\text{CH}_3)_2 \rightarrow \text{cis-CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CHCH}_3$							
1,3-Pentadiene, 3,4-dimethyl- → 1,3-Pentadiene, 2,3-dimethyl-, (Z)-							
71 FRE/LAM Thermal isomerization in a static system. Gas-chromatography. k is P-independent between 0.75 and 7.5 torr. k determined from Equilibrium constant and the sum (k _f + k _r).	DE	473-517	1.35(11)	0	17032±108	1	1.26

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
 $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}=\text{CH}_2 + \text{CH}_2=\text{CH}_2$						
Cyclohexene, 1-methyl-						
78 SIM	EX 1000-1180		3.72(15)	0	35000	1
Single-pulse shock-tube.						
 $\rightarrow$ 	(a)					
 $\rightarrow$ 	(b)					
(racemic mixture)						
$\rightarrow$ trans,trans- $\text{CH}_3\text{CH}=\text{CHCH}=\text{CHCH}_2\text{CH}_3$	(c)					
$\rightarrow$ trans,cis- $\text{CH}_3\text{CH}=\text{CHCH}=\text{CHCH}_2\text{CH}_3$	(d)					
$\rightarrow$ cis,trans- $\text{CH}_3\text{CH}=\text{CHCH}=\text{CHCH}_2\text{CH}_3$	(e)					
$\rightarrow \text{CH}_3\text{CH}_2\text{C}\equiv\text{CCH}_2\text{CH}_2\text{CH}_3$	(f)					
Cyclopropene, 1,3-diethyl-, (-)-						
$\rightarrow$ Cyclopropene, 1,3-diethyl-, (+)-	(a)					
$\rightarrow$ Cyclopropene, 1,3-diethyl-, ($\pm$)-	(b)					
$\rightarrow$ 2,4-Heptadiene- (E,E)-	(c)					
$\rightarrow$ 2,4-Heptadiene- (E,Z)-	(d)					
$\rightarrow$ 2,4-Heptadiene- (Z,E)-	(e)					
$\rightarrow$ 3-Heptyne	(f)					
73 YOR/DIT ¹⁾	EX 434-463		3.16(11)	0	16457 $\pm$ 755	1 10.0
k_A .						
Isomerization to the enantiomer.						
73 YOR/DIT ¹⁾	EX 434-463		6.31(11)	0	16407 $\pm$ 755	1 10.0
k_B .						
Racemization.						
(Loss of optical activity.)						
73 YOR/DIT ¹⁾	EX 434-463		2.51(10)	0	16205 $\pm$ 755	1 10.0
$k_C + k_D + k_E + k_F$, or $k_C + k_D + k_E$,						
according to the mechanism proposed						
in scheme V, or VI, respectively.						
Isomerization by decyclization.						
¹⁾ Static reactor pyrolysis.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 Cyclopropene, 1,3-diethyl-, (+)- → Cyclopropene, 1,3-diethyl-, (-)- (a) → Cyclopropene, 1,3-diethyl-, (±)- (b) → 2,4-Heptadiene- (E,E)- (c) → 2,4-Heptadiene- (E,Z)- (d) → 2,4-Heptadiene- (Z,E)- (e) → 3-Heptyne (f)							
73 YOR/DIT ¹⁾ k _a . Isomerization to the enantiomer.	EX	434-463	3.16(11)	0	16457±755	1	10.0
73 YOR/DIT ¹⁾ k _b . Racemization.	EX	434-463	6.31(11)	0	16407±755	1	10.0
73 YOR/DIT ¹⁾ k _c + k _d + k _e + k _f , or k _c + k _d + k _e , according to the mechanism proposed in scheme V, or VI, respectively. Isomerization by decyclization.	EX	434-463	2.51(10)	0	16205±755	1	10.0
¹⁾ Static reactor pyrolysis.							
 Bicyclo[4.1.0]heptane → Cycloheptene (a) → Cyclohexane, methylene- (b) → Cyclohexene, 1-methyl- (c)							
73 FLO/PEN2 ¹⁾ k _a . Isomerization.	EX	708-769	6.61(14)	0	32662±503	1	1.91

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
73 FLO/PEN2 ¹⁾ k _b . Isomerization.	EX	708-769	1.20(15)	0	33166±705	1	2.69
73 FLO/PEN2 ¹⁾ k _c . Isomerization.	EX	708-769	9.5(14)	0	32511±856	1	3.16
¹⁾ Thermolysis in a static system. P ~ 4.5 torr.							
CH ₃ CH ₂ CH ₂ CH ₂ CH=CH ₂ → products							
1-Heptene							
74 MAG/IOA	EX	823-923	3.55(13)	0	28334	1	
cis-CH ₃ CH ₂ CH ₂ CH ₂ CH=CHCH ₃ → trans-CH ₃ CH ₂ CH ₂ CH ₂ CH=CHCH ₃							
2-Heptene, (Z)-							
74 BAU/YAD	RL	1000-1150	1.0	0	0	1/1	
Rate-ratio assumed to be T-independent. k _{ref} : cis-CH ₃ CH=CHCH ₃ → trans-CH ₃ CH=CHCH ₃							
(CH ₃) ₂ CHCH=C(CH ₃) ₂ → (CH ₃) ₂ CCH=CHCH ₃ + CH ₃ (a) → (CH ₃) ₂ C=CHCHCH ₃ + CH ₃ (b)							
2-Pentene, 2,4-dimethyl-							
73 TSA1	EX	1077-1151	~1.0(16)	0	35050	1	
1,1,2,2-Tetramethylcyclopropane/Cyclohexene/ Toluene/Ar thermolysis in a single-pulse shock-tube. k's determined relative to the decomposition of Cyclohexene. [Tetramethylcyclopropane] = 0.02%. [Cyclohexene] = 0.01%. [Toluene + Ar] = 1%.							
 → CH ₂ =CH ₂ + CH ₃ CH=C(CH ₃) ₂ (a) → CH ₃ CH=CH ₂ + (CH ₃) ₂ C=CH ₂ (b)							
Cyclobutane, 1,1,2-trimethyl-							
→ Ethene + 2-Butene, 2-methyl- (a) → 1-Propene + 1-Propene, 2-methyl- (b)							
71 COC/FRE3 ¹⁾ k _a .	EX	660-728	8.51(15)	0	32149±97	1	1.15
71 COC/FRE3 ¹⁾ k _b .	EX	660-728	5.62(15)	0	30282±116	1	1.17
¹⁾ Pyrolysis in a static system. k is P-independent within this P-range. P > 5 torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\begin{array}{c} \text{H}_3\text{C} \quad \text{CH}_3 \\ \diagdown \quad / \\ \text{C} \\ / \quad \diagdown \\ \text{H}_3\text{C} \quad \text{CH}_3 \end{array} \rightarrow (\text{CH}_3)_2\text{CHCH}=\text{C}(\text{CH}_3)_2$						
Cyclopropane, 1,1,2,2-tetramethyl-						
→ 2-Pentene, 2,4-dimethyl-						
73 TSA1	EX	1077-1151	6.61(14)	0	31320	1
1,1,2,2-tetramethylcyclopropane/Cyclohexene/ Toluene/Ar thermolysis in a single-pulse shock-tube. k's determined relative to the decomposition of Cyclohexene. [Tetramethylcyclopropane] = 0.02%. [Toluene + Ar] = 1 %. [Cyclohexene] = 0.01%.						
$(\text{CH}_3)_2\text{CHCH}_2\text{C}(\text{CH}_3)_2^\dagger \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + (\text{CH}_3)_2\text{CH}$						
Butyl, 1,1,3-trimethyl-						
71 GEO/RAB	EX	298	2.11(7)			1
$(\text{CH}_3)_2\text{CHCH}_2\text{C}(\text{CH}_3)_2^\dagger \text{ formed by:}$ $\text{H} + (\text{CH}_3)_2\text{CHCH}_2\text{C}(\text{CH}_3)=\text{CH}_2$						
$(\text{CH}_3)_3\text{CCH}_2\text{CHCH}_3^\dagger \rightarrow (\text{CH}_3)_3\text{C} + \text{CH}_3\text{CH}=\text{CH}_2$						
Butyl, 1,3,3-trimethyl-						
71 GEO/RAB	EX	298	1.70(8)			1
$(\text{CH}_3)_3\text{CCH}_2\text{CHCH}_3^\dagger \text{ formed by: } \text{H} + (\text{CH}_3)_3\text{CCH}_2\text{CH}=\text{CH}_2$						
$(\text{CH}_3)_2\text{CHC}(\text{CH}_3)_2\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{C}=\text{CH}_2 \quad (\text{a})$ $\rightarrow (\text{CH}_3)_2\text{CHC}(\text{CH}_3)=\text{CH}_2 + \text{CH}_3 \quad (\text{b})$						
Butyl, 2,2,3-trimethyl-						
81 BAL/WAL2 1) 3)	ES	753	(2.4±0.6)(6)			1
81 BAL/WAL2 1) 3)	EX	298-753	6.31(13)	0	12870±842	1 3.16
1) k _a .						
81 BAL/WAL2 2) 3)	RN	753	(2.4±0.6)(5)			1
81 BAL/WAL2 2) 3)	RN	298-753	6.3(13)	0	14554±842	1 3.16
2) k _b .						
3) Oxidation of 2,2,3-Trimethylbutane in H ₂ /O ₂ mixtures, in aged boric-acid-coated reaction vessels. Estimations based on a proposed mechanism. P(Total) = 500 torr. P(2,2,3-Trimethylbutane) = 5 torr.						
$(\text{CH}_3)_3\text{CCH}(\text{CH}_3)\text{CH}_2 \rightarrow (\text{CH}_3)_3\text{C} + \text{CH}_3\text{CH}=\text{CH}_2 \quad (\text{a})$ $\rightarrow (\text{CH}_3)_3\text{CCH}=\text{CH}_2 + \text{CH}_3 \quad (\text{b})$						
Butyl, 2,3,3-trimethyl-						
81 BAL/WAL2 1) 3)	ES	753	1.3(6)			1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 BAL/WAL2 ¹) ³) ¹) k_a .	ES	298-753	6.31(13)	0	13352±842	1	3.16
81 BAL/WAL2 ²) ³)	RN	753	(6.2±3.1)(4)			1	
81 BAL/WAL2 ²) ³) ²) k_b .	RN	298-753	6.31(13)	0	15637±842	1	3.16
³) Oxidation of 2,2,3-Trimethylbutane in H ₂ /O ₂ mixtures, in aged boric-acid-coated reaction vessels. Estimations based on a proposed mechanism. P(Total) = 500 torr. P(2,2,3-Trimethylbutane) = 5 torr.							
$(CH_3)_3CC(CH_3)_2 \rightarrow (CH_3)_2C=CH_2 + (CH_3)_2CH$ (a) $\rightarrow (CH_3)_2C=C(CH_3)_2 + CH_3$ (b)							
Propyl, 1,1,2,2-tetramethyl-							
81 BAL/WAL2 ¹) ²)	RN	753	(7.4±2.5)(5)			1	
81 BAL/WAL2 ¹) ²) ¹) k_a .	RN	298-753	6.31(13)	0	13712±842	1	3.16
²) Oxidation of 2,2,3-Trimethylbutane in H ₂ /O ₂ mixtures, in aged boric-acid-coated reaction vessels. Estimations based on a proposed mechanism. P(Total) = 500 torr. P(2,2,3-Trimethylbutane) = 5 torr.							
80 BAL/WAL k_b . Decomposition of 2,2,3-Trimethylbutane in presence of O ₂ . P = (60-500) torr.	RN	953	1.4(3)			1	
$(CH_3)_3CC(CH_3)_2 + O_2 \rightarrow (CH_3)_3CC(CH_3)=CH_2 + HO_2$ Propyl, 1,1,2,2-tetramethyl- + Oxygen molecule							
80 BAL/WAL k_{ref} : $(CH_3)_3CC(CH_3)_2 \rightarrow (CH_3)_2C=C(CH_3)_2 + CH_3$ Decomposition of 2,2,3-Trimethylbutane in presence of O ₂ . P = (60-500) torr.	RL	773	(9.4±1.8)(7)			2/1	
81 BAL/WAL2 ¹) k_{ref} : $(CH_3)_3CC(CH_3)_2 \rightarrow (CH_3)_2C=CH_2 + (CH_3)_2CH$	RL	753	(1.75±0.20)(5)			2/1	
81 BAL/WAL2 ¹) ¹) Oxidation of 2,2,3-Trimethylbutane in H ₂ /O ₂ mixtures, in aged boric-acid-coated reaction vessels. Estimation based on a proposed mechanism. P(Total) = 500 torr. P(2,2,3-Trimethylbutane) = 5 torr.	RN	753	(1.3±0.2)(11)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃(CH₂)₅CH₃ → products							
Heptane							
73 ILL/WEL	EX	873-1073	(1.89±0.03)(12)	0	26447	1	
75 TAN/KRA	EX	763-813	1.58(10)	0	24660	1	
75 TAN/KRA	EX	763-813	1.6(10)	0	24660	1	
Thermolysis in a static reactor.							
P = (75-150) torr.							
79 BAJ/VES	EX	953-1033	1.3(11)	0	23516	1	
Thermolysis in a tubular flow-reactor.							
P ~ 1 atm.							
(CH₃)₂CHCH₂CH(CH₃)₂ → products							
Pentane, 2,4-dimethyl-							
73 ILL/WEL	EX	873-1073	(4.48±0.12)(14)	0	31228	1	
(CH₃)₃CCH(CH₃)₂ → (CH₃)₃C + (CH₃)₂CH							
Butane, 2,2,3-trimethyl-							
80 BAL/WAL	EX	953-1198	2.88(16)	0	36687±180	1	1.32
Decomposition of 2,2,3-Trimethylbutane							
in presence of O ₂ .							
P = (60-500) torr.							
							
Bicyclo[3.2.0]hept-2-en-6-one							
→ 1,3-Cyclopentadiene + Ethenone							
72 EGG/COC	EX	471-534	1.45(13)	0	18888±126	1	1.29
Pyrolysis in a static system.							
P ₀ = (15-485) torr.							
							
Bicyclo[3.2.0]heptan-6-one → Cyclopentene + Ethenone							
72 COC/EGG4	EX	546-652	1.62(14)	0	24434±146	1	1.26
Pyrolysis in a static system.							
P ₀ = (3.8-40) torr.							
CH₂=C=CHC(CH₃)₂COOH → CH₂=CHCH=C(CH₃)₂ + CO₂							
3,4-Pentadienoic acid, 2,2-dimethyl-							
76 BIG/WEA2	EX	500	2.16(-6)			1	
76 BIG/WEA2	EX	630	6.49(-3)			1	
76 BIG/WEA2	EX	500-695	1.67(11)	0	19455±758	1	2.6
A and B recalculated from the reported data.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)_2\text{COOH} \rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CO}_2$							
3-Butenoic acid, 2,2,3-trimethyl-							
82 ALB/BIG ¹⁾	EX	577	1.2(-2)				1
82 ALB/BIG ¹⁾	EX	~577	1.04(11)	0	17176		1
A and B recalculated from the reported data.							
¹⁾ Pyrolysis in a flow-reactor.							
NMR-spectrometry.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2$							
4-Penten-1-ol acetate							
79 MAR/HER	EX	513-693	6.46(12)	0	24538±541	1	2.29
Pyrolysis in a static system.							
P = (44-282) torr.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}(\text{CH}_3)\text{CH}_2\text{CH}=\text{CH}_2$							
$\rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2$ (a)							
$\rightarrow \text{CH}_3\text{COOH} + \text{CH}_3\text{CH}=\text{CHCH}=\text{CH}_2$ (b)							
4-Penten-2-ol acetate							
79 MAR/HER	EX	513-693	2.19(12)	0	21435±349	1	1.78
$k_a + k_b$.							
Pyrolysis in a static system.							
P = (44-282) torr.							
$\text{trans-CH}_3\text{CH}=\text{CHC}(\text{O})\text{OCH}(\text{CH}_3)_2$							
$\rightarrow \text{trans-CH}_3\text{CH}=\text{CHCOOH} + \text{CH}_3\text{CH}=\text{CH}_2$							
2-Butenoic acid, (E)-, 1-methylethyl ester							
77 SMI/MUT	EX	651	(7.10±0.20)(-3)			1	
HCOO  $\rightarrow \text{CH}_3\text{COOH} +$ 							
Formic acid cyclohexyl ester (Cyclohexyl formate)							
$\rightarrow$ Formic acid + Cyclohexene							
72 TIN/KOO	EX	623-673	1.26(12)	0	21641±1007	1	3.98
Thermolysis.							
CH_3COO  $\rightarrow \text{CH}_3\text{COOH} +$ 							
Cyclopentanol acetate $\rightarrow$ Acetic acid + Cyclopentene							
72 TIN/KOO	EX	588-663	1.58(12)	0	20835±503	1	3.98
Thermolysis.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/(ref), A, A/(ref)	n	B, B-B(ref)	k, A k err. units factor
$\triangle \begin{array}{c} \text{CH}_3 \\ \\ \text{C}-\text{COOH} \\ \\ \text{CH}_3 \end{array} \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{C}(\text{CH}_3)_2 + \text{CO}_2 \quad (\text{a}) = (\text{b})$ $\rightarrow (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{CO}_2 \quad (\text{c})$						
Cyclopropaneacetic acid, α, α -dimethyl-						
$\rightarrow$ 2-Pentene, 2-methyl- + Carbon dioxide (a) = (b)						
$\rightarrow$ 2-Butene, 2,3-dimethyl- + Carbon dioxide (c)						
79 BIG/FET ²)	EX	725	1.31(-3)			1
$k_a = k_b$.						
79 BIG/FET ²)	EX	725	<5.0(-5			1
k_c . Upper-limit k.						
79 BIG/FET ¹) ²)	EX	725	2.62(-3)			1
79 BIG/FET ¹) ²)	EX	690-740	(1.74 $\pm$ 0.07)(11)	0	23074 $\pm$ 349	1
A and B recalculated from the reported data.						
¹) $k_a + k_b + k_c$.						
²) Pyrolysis in a Flow-reactor with evacuated sealed tubes.						
Gas-chromatography. NMR-spectroscopy.						
$\text{H}_3\text{C} \triangle \text{CH}_2\text{COOH} \rightarrow (\text{CH}_3)_3\text{CCH}=\text{CH}_2 + \text{CO}_2 \quad (\text{a})$ $\rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}=\text{CH}_2 + \text{CO}_2 \quad (\text{b})$ $\rightarrow (\text{CH}_3)_2\text{CHC}(\text{CH}_3)=\text{CH}_2 + \text{CO}_2 \quad (\text{c})$						
Cyclopropaneacetic acid, 2,2-dimethyl-						
$\rightarrow$ 1-Butene, 3,3-dimethyl- + Carbon dioxide (a)						
$\rightarrow$ 1-Pentene, 4-methyl- + Carbon dioxide (b)						
$\rightarrow$ 1-Butene, 2,3-dimethyl- + Carbon dioxide (c)						
80 BIG/FET ²)	EX	725	8.2(-4)			1
k_a .						
80 BIG/FET ²)	EX	725	4.8(-4)			1
k_b .						
80 BIG/FET ²)	EX	725	1.0(-4)			1
k_c .						
80 BIG/FET ¹) ²)	EX	725	1.4(-3)			1
80 BIG/FET ¹) ²)	EX	750-820	4.49(11)	0	24215 $\pm$ 722	1
A and B recalculated from the reported data.						
¹) $k_a + k_b + k_c$.						
²) Pyrolysis in a flow-reactor with evacuated sealed tubes.						
Gas-chromatography. NMR-spectrometry.						
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{C}(\text{O})\text{CH}_3$						
2-Pentanone, 5-acetyloxy-						
76 DEB/TAY	EX	650-700	6.31(12)	0	23905	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k _A units	k err. factor
CH₃C(O)OC(CH₃)₂C(O)CH₃ → CH₃COOH + CH₂=C(CH₃)C(O)CH₃							
2-Butanone, 3-(acetyloxy)-3-methyl-							
76 CHU/MAR ¹⁾	EX	573	9.54(-4)			1	
76 CHU/MAR ¹⁾	EX	543-593	2.88(13)	0	21741±201	1	1.48
¹⁾ Thermolysis in a clean or seasoned Pyrex vessel.							
P = (69-222) torr.							
CH₃C(O)OC(CH₃)₂C(O)OCH₃ → CH₃COOH + CH₂=C(CH₃)C(O)OCH₃							
Propanoic acid, 2-(acetyloxy)-2-methyl-, methyl ester							
80 MAR/CHU	EX	503-613	3.39(12)	0	21182±433	1	2.09
Pyrolysis in a static system. Mass-spectrometry.							
IR-, and NMR-spectroscopy.							
P = (56-210) torr.							
$ \begin{array}{c} \text{O} \\ \parallel \\ \text{H}_3\text{C}_2\text{C}-\text{C}-\text{C} \\ \parallel \quad \parallel \\ \text{H}_3\text{C}_2\text{C} \quad \text{H}_3\text{C}_2\text{C} \end{array} \rightarrow \text{HCHO} + (\text{CH}_3\text{CH}_2)_2\text{C}=\text{CH}_2 $							
Oxetane, 3,3-diethyl-							
→ Formaldehyde + Pentane, 3-methylene-							
75 CLE/FRE	EX	675-736	1.98(15)	0	30053±101	1	1.16
Thermolysis in a static system.							
CH₃C(O)OCH₂CH₂CH(CH₃)₂ → CH₃COOH + CH₂=CHCH(CH₃)₂							
1-Butanol, 3-methyl-, acetate							
79 CHU/MAR	EX	633-693	5.37(12)	0	24358±457	1	1.95
Pyrolysis in a static system.							
P = (63-250) torr.							
79 TAY	EX	660-712	6.61(12)	0	24509	1	
Pyrolysis in a stainless-steel reactor.							
CH₃C(O)OCH₂CH₂CH(CH₃)₂ + O₂(a¹Δ_g) → products							
1-Butanol, 3-methyl-, acetate + Oxygen molecule							
79 DAT/RAO	EX	298	(5.2±1.1)(6)			2	
Microwave discharge flow system.							
CH₃C(O)OC(CH₃)₂CH₂CH₃ → CH₃COOH + (CH₃)₂C=CHCH₃ (a)							
→ CH₃COOH + CH₃CH₂C(CH₃)=CH₂ (b)							
2-Butanol, 2-methyl-, acetate							
72 TIN/KOO	EX	535-596	1.58(12)	0	19376±503	1	2.51
k _a . Thermolysis.							
72 TIN/KOO	EX	535-596	5.01(12)	0	19376±503	1	2.51
k _b . Thermolysis.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{C}(\text{O})\text{OCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2$							
→ $\text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}(\text{CH}_3)_2$ (a)							
→ $\text{CH}_3\text{COOH} + \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2$ (b)							
2-Butanol, 3-methyl-, acetate							
73 CHU/MAR	EX	583-643	1.33(13)	0	22934±242	1	1.01
$k_a + k_b$.							
Pyrolysis in a static system.							
Channel (a) is predominant.							
P = (30-300) torr.							
$(\text{CH}_3)_2\text{CHC}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CHCOOH} + \text{CH}_3\text{CH}=\text{CH}_2$							
Propanoic acid, 2-methyl-, 1-methylethyl ester							
77 SMI/MUT	EX	651	(6.80±0.20)(-3)			1	
$\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OC}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{CH}_2\text{COOH} + (\text{CH}_3)_2\text{C}=\text{CH}_2$							
Propanoic acid 1,1-dimethylethyl ester							
78 TAY	EX	543-620	3.63(12)	0	19341	1	
Pyrolysis in a stainless-steel reactor.							
$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$							
Butanoic acid 1-methylethyl ester							
77 SMI/MUT	EX	651	(5.93±0.27)(-3)			1	
78 CHU/MAR ¹⁾	EX	603	4.07(-4)			1	
78 CHU/MAR ¹⁾	EX	583-622	2.45(13)	0	23301±252	1	1.58
¹⁾ Pyrolysis in a static system.							
$\text{CH}_3\text{CH}_2\text{CH}_2\text{OC}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_3$							
→ $\text{CH}_3\text{CH}=\text{CH}_2 + \text{CO}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$							
Carbonic acid dipropyl ester (Di-n-propyl carbonate)							
72 BIG/WRE1 ¹⁾	EX	700	(7.35±0.22)(-2)			1	
72 BIG/WRE1 ¹⁾	EX	663-708	(4.02±0.12)(13)	0	23754	1	
The A-factor recalculated from the reported experimental data.							
¹⁾ Pyrolysis in the Kooyman flow-tube.							
72 BIG/WRE3	EX	629	1.42(-3)			1	
Flow-tube method.							
76 CRO/HUN	EX	583-667	9.33(11)	0	21892	1	
$(\text{CH}_3)_2\text{CHOC}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CO}_2 + (\text{CH}_3)_2\text{CHOH}$							
Carbonic acid bis(1-methylethyl) ester							
(Di-i-propyl carbonate)							
72 BIG/WRE2 ¹⁾	EX	629	3.99(-2)			1	

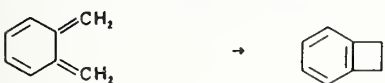
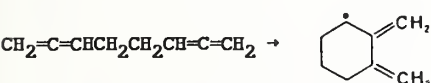
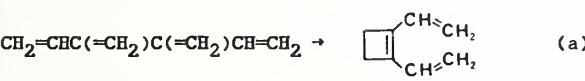
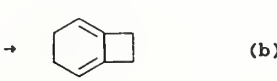
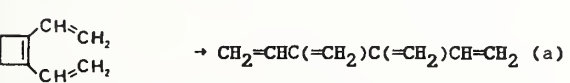
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
72 BIG/WRE2 ¹⁾ The A-factor recalculated from the reported data.	EX	593-648	2.20(14)	0	22798	1
¹⁾ Flow-tube pyrolysis.						
$(\text{CD}_3)_2\text{CHOC}(\text{O})\text{CH}(\text{CD}_3)_2 \rightarrow \text{CD}_3\text{CH}=\text{CD}_2 + \text{CO}_2 + (\text{CD}_3)_2\text{CHOD}$						
Carbonic acid bis(1-methyl-d ₃ -ethyl-2,2,2-d ₃) ester						
72 BIG/WRE2 ¹⁾	EX	629	1.66(-2)			1
72 BIG/WRE2 ¹⁾	EX	593-648	2.39(14)	0	23402	1
The A-factor recalculated from the reported data.						
¹⁾ Flow-tube pyrolysis.						
$\text{CH}_3\text{OCH}_2\text{C}(\text{O})\text{OC}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{OCH}_2\text{COOH} + (\text{CH}_3)_2\text{C}=\text{CH}_2$						
Acetic acid, methoxy-, 1,1-dimethylethyl ester						
78 TAY	EX	528-587	3.09(13)	0	20232	1
Pyrolysis in a stainless-steel reactor.						
Gas-chromatography.						
$\text{CH}_3\text{OC}(\text{O})\text{OC}(\text{CH}_3)_2\text{CH}_2\text{CH}_3$						
$\rightarrow \text{CH}_3\text{OH} + \text{CO}_2 + \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3$ (a)						
$\rightarrow \text{CH}_3\text{OH} + \text{CO}_2 + (\text{CH}_3)_2\text{C}=\text{CHCH}_3$ (b)						
Carbonic acid						
1,1-dimethylpropyl methyl ester						
72 BIG/WRE3	EX	629	3.48			1
72 BIG/WRE3	EX	593-648	3.97(12)	0	17464	1
k _a + k _b .						
Flow-tube method.						
Assumed T-range, omitted in text.						
The A-factor recalculated from the reported data.						
$\text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{OOH} \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{O} + \text{OH}$						
Hydroperoxide, heptyl- → Heptoxy + Hydroxyl						
80 SAH/HEI	EX	540-625	≈3.0(15)	0	21750±500	1
Decomposition in a Pyrex reactor						
with continuous flow.						
Gas-chromatography.						
P = 100 torr.						
82 SAH/HEI1	EX	523-633	(1.10±0.25)(16)	0	21892±503	1
Decomposition in a flow system, in a mixture						
containing O ₂ , H ₂ and CO ₂ . Thin-layer and						
liquid-phase Gas-chromatography.						
[Hydroperoxide] = 1.23x10 ¹⁸ molec.cm ⁻³ .						
P = 100 torr.						

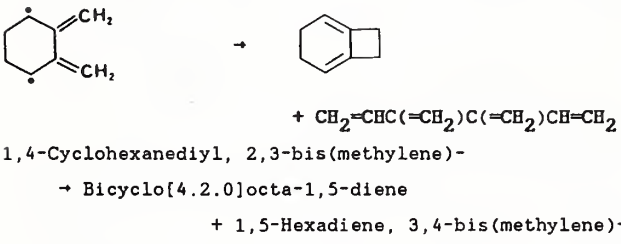
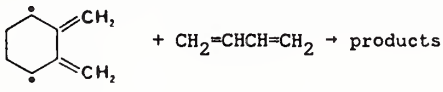
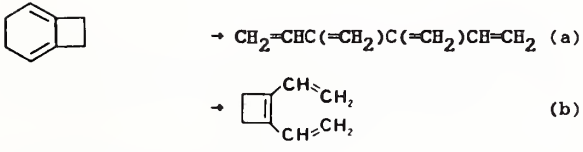
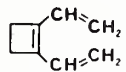
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{OOH})\text{CH}_3 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{O}\cdot)\text{CH}_3 + \text{OH}$							
Hydroperoxide, 1-methylhexyl-							
82 SAN/HEI1 Decomposition in a flow system, in a $\text{O}_2/\text{H}_2/\text{CO}_2$ mixture. Thin-layer and liquid-phase Gas-chromatography. [Hydroperoxide] = 1.23×10^{18} molec. cm^{-3} . P = 100 torr.	EX	523-633	(7.0 $\pm$ 2.0)(15)	0	20886 $\pm$ 503	1	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{SCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CHS} + \text{CH}_3\text{CH}=\text{CH}_2$							
Butane, 1-(2-propenylthio)- $\rightarrow$ Butanethial + 1-Propene							
82 MAR/DRA Pyrolysis in a static system. Gas-chromatography. NMR-, and Mass-spectrometry. Butanethial trimerizes to the cyclic compound 2,4,6-Tripropyl-1,3,5-trithiane. P ₀ = (87-685) torr.	EX	535-566	2.63(11)	0	18644 $\pm$ 361	1	1.91
$(\text{CH}_3)_3\text{CN}=\text{NCH}_2\text{CH}=\text{CH}_2 \rightarrow (\text{CH}_3)_3\text{C} + \text{CH}_2\text{CH}=\text{CH}_2 + \text{N}_2$							
Diazene, (1,1-dimethylethyl)-2-propenyl-							
72 CRA/TAK Thermolysis. Mass-spectrometry. Gas-chromatography. In presence of ^{15}NO . P(Total) = (50-60) torr.	EX	354-399	5.37(12)	0	14997 $\pm$ 151	1	1.82
$(\text{CH}_3)_2\text{NC}(\text{O})\text{OC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_2\text{NH} + \text{CO}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2$							
Carbamio acid, dimethyl-, 1,1-dimethylethyl ester							
72 DAL/ZIO2 Thermolysis in a conventional static system.	EX	323-333	7.41(12)	0	18993 $\pm$ 201	1	
72 KWA/SLU Thermolysis in a conventional static system.	EX	575-636	1.86(13)	0	19628 $\pm$ 50	1	1.07
$(\text{CH}_3)_2\text{NC}(\text{O})\text{OC}(\text{CD}_3)_3 \rightarrow (\text{CH}_3)_2\text{ND} + \text{CO}_2 + (\text{CD}_3)_2\text{C}=\text{CD}_2$							
Carbamic acid, dimethyl-, (1,1-dimethyl-d ₃) ester							
72 KWA/SLU Thermolysis in a conventional static system.	EX	584-647	2.34(13)	0	20282 $\pm$ 50	1	1.12

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

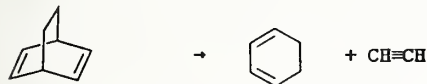
Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
 1,3-Cyclohexadiene, 5,6-bis(methylene)- → Bicyclo[4.2.0]octa-1,3,5-triene	EX	594-757	(2.1±1.1)(12)	0	13538±352	1
81 ROT/SCH Thermal isomerization behind incident shock-waves in N ₂ , or He as carrier gas. UV-spectrometry.						
 1,2,6,7-Octatetraene → 1,4-Cyclohexanediyl, 2,3-bis(methylene)-	EX	369-455	(6.1±0.8)(9)	0	12380±50	1
82 ROT/SCH2 Thermal rearrangement in an air thermostat. P = (5.3-585) torr.						
 1,5-Hexadiene, 3,4-bis(methylene)- → Cyclobutene, 1,2-diethenyl- (a)						
 → Bicyclo[4.2.0]octa-1,5-diene (b)						
82 ROT/SCH2 1) k _a .	EX	495-549	(2.5±1.3)(11)	0	17967±252	1
82 ROT/SCH2 1) k _b .	EX	495-549	(2.4±1.0)(10)	0	16960±201	1
1) Thermal rearrangement in an air thermostat. P = (5.3-585) torr.						
 Cyclobutene, 1,2-diethenyl- → 1,4-Hexadiene, 3,4-bis(methylene)- (a)						
 → Bicyclo[4.2.0]octa-1,5-diene (b)						
82 ROT/SCH2 k _a .	EX	424-479	(4.8±0.7)(13)	0	17967±50	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 ROT/SCH2 k_b . Thermal rearrangement in an air thermostat. P = 5.3-585) torr.	EX	424-479	(3.0±0.8)(11)	0	14947±101	1	
 1,4-Cyclohexanediyl, 2,3-bis(methylene)- → Bicyclo[4.2.0]octa-1,5-diene + 1,5-Hexadiene, 3,4-bis(methylene)-							
82 ROT/SCH1 Thermal rearrangement in an air thermostat.	RL	318-356	(7.4±8.9)(2)	0	5788±403	1/2	
k_{ref} :  + CH₂=CHCH=CH₂ → products							
 → CH₂=CHC(=CH₂)C(=CH₂)CH=CH₂ (a) →  (b)							
Bicyclo[4.2.0]octa-1,5-diene → 1,5-Hexadiene, 3,4-bis(methylene)- (a) → Cyclobutene, 1,2-diethenyl- (b)							
82 ROT/SCH2 ¹⁾ k_a .	EX	486-518	(2.4±1.3)(14)	0	21087±252	1	
82 ROT/SCH2 ¹⁾ k_b .	EX	495-549	(1.6±0.3)(13)	0	19124±50	1	
¹⁾ Thermal rearrangement in an air thermostat. P = (5.3-585) torr.							
 Bicyclo[2.2.0]hexane, 2,3-bis(methylene)- → 1,4-Cyclohexanediyl, 2,3-bis(methylene)-							
82 ROT/SCH1 Thermal rearrangement in an air thermostat.	EX	318-368	(8.8±2.1)(12)	0	12984±101	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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Bicyclo[2.2.2]octa-2,5-diene →

1,3-Cyclohexadiene + Ethyne

82 HUY/LEE

EX 354-435

1.14(14)

0

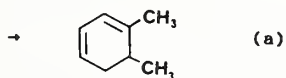
16366±20

1

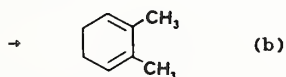
1.05

Thermolysis. Static system.

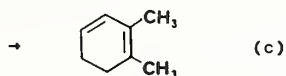
P = (0.5-6.0) torr.

trans,trans,trans-CH₃CH=CHCH=CHCH=CHCH₃

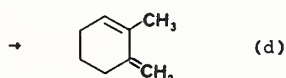
(a)



(b)



(c)



(d)

→ any other products (e)

2,4,6-Octatriene, (E,E,E)-

→ 1,3-Cyclohexadiene, 1,6-dimethyl- (a)

→ 1,3-Cyclohexadiene, 2,3-dimethyl- (b)

→ 1,3-Cyclohexadiene, 1,2-dimethyl- (c)

→ Cyclohexene, 1-methyl-6-methylene- (d)

→ other products (e)

73 DOE/BEA

EX 533-583

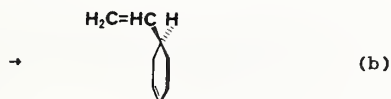
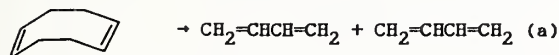
2.89(13)

0

22748±327

1

1.78

k_{overall}. Thermal isomerization.

(b)

1,5-Cyclooctadiene, (Z,Z)-

→ 1,3-Butadiene (a)

→ Cyclohexene, 4-ethenyl- (b)

72 DOE/FRA¹⁾

EX 575-630

2.00(16)

0

28148±468

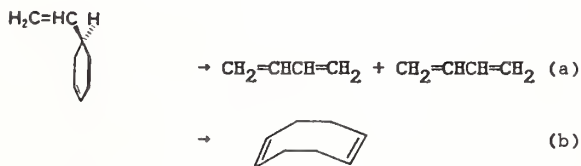
1

1.86

k_a. Thermal dissociation.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 HUY/LUY ²⁾ k _a . Thermal dissociation.	EX	505-586	2.88(16)	0	28374±50	1	1.10
72 DOE/FRA ¹⁾ k _b . Thermal rearrangement.	EX	575-630	3.55(15)	0	26371±574	1	2.19
77 HUY/LUY ²⁾ k _b . Thermal rearrangement.	EX	505-586	2.19(15)	0	26059±60	1	1.12
72 DOE/FRA ¹⁾ k _a + k _b . Overall reaction.	EX	575-630	9.77(15)	0	26819±382	1	1.70
¹⁾ Pyrolysis in a 3.5 l. lead-potash glass vessel.							
²⁾ Thermal reaction. Static system.							
P = (15-51) torr.							

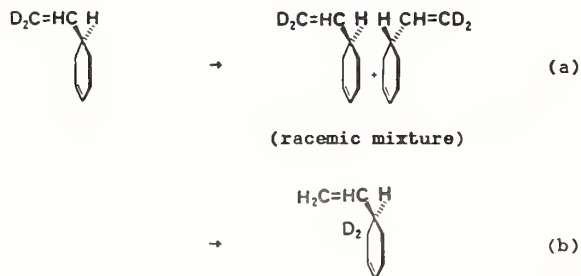


Cyclohexene, 4-ethenyl-

→ 1,3 Butadiene (a)

→ 1,5-Cyclooctadiene, (Z,Z)- (b)

77 HUY/LUY ¹⁾ k _a . (k _a = k _{-a} K.)	DE	464-557	2.51(14)	0	30297±252	1	3.16
77 HUY/LUY ¹⁾ k _b . (k _b = k _{-b} K.)	DE	464-557	7.94(13)	0	29995±352	1	3.16

¹⁾ Thermal reaction of 1,3-Butadiene
and 1,5-Cyclooctadiene. Static system.

Cyclohexene, 4-(ethenyl-2,2-d₂)-, (R)-

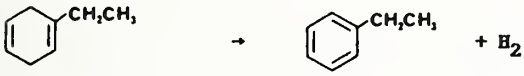
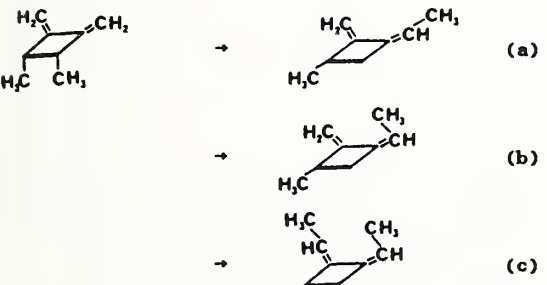
→ Cyclohexene, 4-(ethenyl-2,2-d₂)-, (±)- (a)

→ Cyclohexene-3,3-d₂, 4-ethenyl- (b)

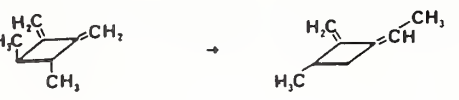
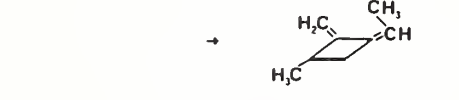
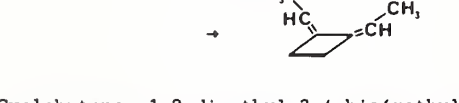
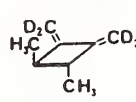
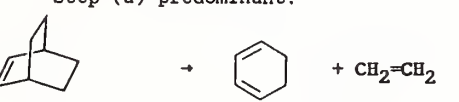
72 DOE/FRA ¹⁾ k _a . Thermal racemization.	EX	575-630	1.23(12)	0	24987±400	1	1.82
72 DOE/FRA ¹⁾ k _b . Thermal rearrangement.	EX	575-630	1.23(13)	0	26241±896	1	4.17

¹⁾ Pyrolysis in a 12 liter Pyrex vessel.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 1,4-Cyclohexadiene, 1-ethyl- → Benzene, ethyl- + Hydrogen molecule 72 COC/FRE Pyrolysis in a static system. P₀ = 10 torr.	EX	589-652	1.32(13)	0	23085±126	1	1.23
 1,4-Cyclohexadiene, 1,2-dimethyl- → Benzene, 1,2-dimethyl- (o-Xylene) + Hydrogen molecule 72 COC/FRE Pyrolysis in a static system. P₀ = (3-4) torr.	EX	572-627	3.47(12)	0	22003±40	1	1.07
 Cyclobutane, 1,2-diethenyl-, trans- → products 81 GRI/SCH Thermal rearrangement in an air thermostat. P = (2-3) torr.	EX	448-503	(1.93±0.31)(13)	0	17861±75	1	
 Cyclobutane, 1,2-dimethyl-3,4-bis(methylene)-, cis- → Cyclobutane, 1-ethylidene-3-methyl- 2-methylene-, (E)- (a) → Cyclobutane, 1-ethylidene-3-methyl- 2-methylene-, (Z)- (b) → Cyclobutane, 1,2-diethylidene-, (E,Z)- (c) 82 GAJ/BEN k_a + k_b + k_c. Thermal isomerization in a flow-reactor. Channel (b) predominant.	EX	588-648	5.01(13)	0	21238	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
  							
Cyclobutane, 1,2-dimethyl-3,4-bis(methylene)-, trans-							
→ Cyclobutane, 1-ethylidene-3-methyl-2-methylene-, (E)- (a)							
→ Cyclobutane, 1-ethylidene-3-methyl-2-methylene-, (Z)- (b)							
→ Cyclobutane, 1,2-diethylidene-, (E,E)- (c)							
82 GAJ/BEN 1) 2)	EX	588-648	3.98(13)	0	21087	1	
82 GAJ/BEN 1) 2)	EX	503	2.31(-5)			1	
1) $k_a + k_b + k_c$.							
82 GAJ/BEN 2)	EX	503	(1.08±0.01)			1/1	
$(k_a + k_b + k_c)/k_{ref}$.							
k_{ref} :  → products. (Isotope effect)							
2) Thermal isomerization in a flow-reactor.							
Step (a) predominant.							
							
Bicyclo[2.2.2]oct-2-ene → 1,3-Cyclohexadiene + Ethene							
71 COC/FRE1	EX	649-718	2.88(15)	0	29398±81	1	1.12
Retrodiene thermolysis in a static system.							
Gas. chromatography. P-independent above 4 torr.							
80 HUY/RIG	EX	548-632	1.32(15)	0	28837±50	1	1.10
Retro-Diels-Alder pyrolysis of Bicyclo[2.2.2]oct-2-ene in a static system.							
Gas-chromatography.							
$CH_3C\equiv CCH_2CH_2CH(CH_3)_2 \rightarrow CH_3C\equiv CCH_2 + CH_2CH(CH_3)_2$ (a) $\rightarrow CH_3CH=C=CH_2 + CH_2=C(CH_3)_2$ (b)							
2-Heptyne, 6-methyl-							
78 TSA3 1)	EX	990-1200	1.58(16)	0	36800±500	1	1.61
k_a . Bond-breaking reaction.							

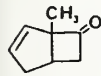
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 TSA3 ¹⁾ k _b . Molecular reaction.	EX	990-1200	2.00(12)	0	28700±1000	1	2.51
¹⁾ 6-Methyl-2-heptyne/Cyclohexene/Toluene/Ar thermolysis in a single-pulse shock-tube. k's determined relative to the decomposition of Cyclohexene. Similar data given in 76 TSA2. [Cyclohexene] = 0.01%. [Toluene] = 1%. [6-Methyl-2-heptyne] = 0.02%. P(Ar) ~ (2-6) atm.							
CH ₃ CH ₂ CH(CH ₃)CH ₂ C(CH ₃)=CH ₂ → CH ₃ CH ₂ CH=CH ₂ + (CH ₃) ₂ C=CH ₂ (a) → CH ₃ CH ₂ CHCH ₃ + CH ₂ C(CH ₃)=CH ₂ (b)							
1-Hexene, 2,4-dimethyl-							
73 TSA2 ¹⁾ ²⁾	EX	996-1180	2.82(12)	0	26900±250	1	1.38
78 TSA5 ¹⁾ ²⁾	EX	996-1180	3.16(12)	0	26900	1	
¹⁾ k _a . 1050 K given by the author as central-T.							
73 TSA2 ²⁾	EX	1050	4.27(15)	0	33200±150	1	1.17
k _b . ²⁾ Single-pulse shock-tube.							
(CH ₃) ₃ CC(CH ₃) ₂ CH ₂ → (CH ₃) ₃ C + (CH ₃) ₂ =CH ₂ (a) → (CH ₃) ₃ CC(CH ₃)=CH ₂ + CH ₃ (b)							
Butyl, 2,2,3,3-tetramethyl-							
79 BAL/WAL2 ¹⁾ k _b /k _a .	RL	753	5.77(-3)				1/1
79 BAL/WAL2 ¹⁾ k _a .	RN	753	1.88(6)				1
79 BAL/WAL2 ¹⁾ k _b .	RN	753	1.08(4)				1
¹⁾ Oxidation in aged boric-acid-coated vessels. Gas-chromatography. Absolute k's determined on the basis of Benson's additivity rules.							
CH ₃ (CH ₂) ₆ CH ₃ → products							
Octane							
73 ILL/WEL	EX	873-1073	(1.04±0.02)(12)	0	26336	1	
80 RUM/SHE	EX	893-993	4.07(13)	0	29867±1516	1	4.90
Pyrolysis in a quartz reactor. P = 760 torr.							
(CH ₃) ₂ CH(CH ₂) ₄ CH ₃ → products							
Heptane, 2-methyl-							
73 ILL/WEL	EX	873-1046	(1.52±0.04)(13)	0	28143	1	

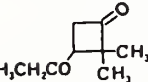
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_3\text{CC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_3\text{C} + (\text{CH}_3)_3\text{C} \quad (\text{a})$ $\rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + (\text{CH}_3)_3\text{CH} \quad (\text{b})$						
Butane, 2,2,3,3-tetramethyl- (Hexamethylethane)						
74 GOL/ALF k_a . Best fit of experimental data to $\log A = 16.4$ for each C-C fission.	DE	850-1150	2.51(16)	0	34222	1
78 ATR/BAL ¹⁾ k_a .	EX	985	2.37(1)			1
78 ATR/BAL ¹⁾ k_a .	EX	1141	2.75(3)			1
78 ATR/BAL ¹⁾ k_a . Based on the above data combined with those from 78 TSA4.	SE	713-813	6.03(16)	0	34931±180	1 1.36
¹⁾ Oxidation in KCl-coated vessels. P = (60-500) torr.						
78 TSA4 ²⁾ k_a .	EX	990-1100	2.51(16)	0	34400	1
78 TSA4 ²⁾ k_a . Extrapolation over the given T-range.	EX	300-1100	2.00(17)	0	36600	1
²⁾ Single-pulse shock-tube.						
79 WAL/TSA k_a . Thermolysis of 6-Methyl-2-heptyne in a flow-system, in He, in presence of 1-Methyl-cyclohexene and Toluene. k 's determined relative to the decomposition of 1-Methylcyclohexene. [1-Methylcyclohexene] = (0.08-0.12)%. [Hexamethylethane] = (0.003-0.04)%. [Toluene] = (2.0-13.6)%.	EX	700-900	2.51(17)	0	36300±200	1 1.58
82 BAL/HIS k_a . Decomposition of Hexamethylethane in KCl-coated-, or Pyrex-aged-boric- acid-coated vessels. Gas-chromatography. P = (1.0-4.0) torr.	EX	673-815	1.04(17)	0	35448±361	1
78 BAL/EVA k_b . Decomposition in cylindrical KCl-coated Pyrex vessels. P = (60-500) torr.	EX	693-813	7.76(13)	0	33078±168	1 1.26
78 TAY/MIL k_{total} . Pyrolysis in wal-less reactor. The products are: 2-Methylpropene, Hydrogen, 1-Propene, 2-Methyl-2-butene, Ethane, Methane, Neopentane and 2,3-Dimethyl-2-butene, in order of abundance.	EX	750-950	5.01(10)	0	21741	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 $\rightarrow$ products							
Bicyclo[3.2.0]hept-3-en-6-one, 5-methyl-							
72 COC/EGG3 Pyrolysis in a static system. Gas-chromatography. P = (2.7-20) torr.	EX	489-565	3.16(14)	0	22108±337	1	1.91
$\text{CH}_2=\text{CH}=\text{CH}_2\text{OC}(\text{O})\text{C}(\text{O})\text{OCH}_2\text{CH}=\text{CH}_2 \rightarrow 2\text{CO}_2 + 2\text{CH}_2=\text{CHCH}_2$ Ethanedioic acid di-2-propenyl ester							
76 SAK/NOH Pyrolysis in a flow-reactor.	EX	723-763	7.94(10)	0	21741	1	
80 NOH/SAK ¹⁾	EX	703-783	2.00(10)	0	22610	1	
81 NOH/SAK ¹⁾	EX	723-783	6.31(10)	0	21651	1	
¹⁾ Pyrolysis in a flow-reactor. Gas-chromatography. Mass-spectrometry.							
$\text{CH}_2=\text{CHCH}=\text{CHC}(\text{CH}_3)_2\text{COOH} \rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}=\text{C}(\text{CH}_3)_2 + \text{CO}_2$ 3,5-Hexanedioic acid, 2,2-dimethyl-							
76 BIG/WEA2	EX	500	7.35(-8)			1	
76 BIG/WEA2	EX	692	2.90(-2)			1	
76 BIG/WEA2 A and B recalculated from the reported data.	EX	500-723	1.42(13)	0	23389±758	1	
$\text{CH}_2=\text{CHCH}=\text{CHC}(\text{CH}_3)_2\text{COOD} \rightarrow \text{CH}_2=\text{CHCHDCH}=\text{C}(\text{CH}_3)_2 + \text{CO}_2$ 3,5-Hexanedioic acid-d, 2,2-dimethyl-							
76 BIG/WEA2	EX	692	1.34(-2)			1	
CH_3COO  $\rightarrow \text{CH}_3\text{COOH} +$  (a)							
$\rightarrow \text{CH}_3\text{COOH} +$  (b)							
3-Cyclohexen-1-ol acetate							
$\rightarrow$ Acetic acid + 1,3-Cyclohexadiene (a)							
$\rightarrow$ Acetic acid + 1,4-Cyclohexadiene (b)							
72 TIN/KOO ¹⁾ $k_a + k_b$.	EX	578-653	3.98(11)	0	19527±503	1	2.0
72 TIN/KOO ¹⁾ k_b/k_a .	RL	637	1.3(1)			1/1	
¹⁾ Thermolysis.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ $\rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CH}_2$							
5-Hexen-1-ol acetate							
79 MAR/HER	EX	513-693	2.69(12)	0	23756±217	1	1.38
Pyrolysis in a static system.							
P = (44-282) torr.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}=\text{C}(\text{CH}_3)_2$ $\rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}=\text{C}(\text{CH}_3)_2$ (a) $\rightarrow \text{CH}_3\text{COOH} + \text{cis-CH}_3\text{CH}=\text{CHC}(\text{CH}_3)=\text{CH}_2$ (b) $\rightarrow \text{CH}_3\text{COOH} + \text{trans-CH}_3\text{CH}=\text{CHC}(\text{CH}_3)=\text{CH}_2$ (c) $\rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ (d)							
3-Penten-1-ol, 4-methyl-, acetate							
81 CHU/MAR	EX	603-653	1.62(13)	0	24008±204	1	1.38
$k_a + k_b + k_c + k_d$. Pyrolysis. Static system.							
IR-, and NMR-spectrometry. P = (53-210) torr.							
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{CH}_2\text{CH}=\text{CH}_2$ $\rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{C}(\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2)$ (a) $\rightarrow \text{CH}_3\text{C}(\text{O})\text{H} + (\text{CH}_3)_2\text{C}=\text{CHCH}=\text{CH}_2$ (b)							
4-Penten-2-ol, 2-methyl-, acetate							
79 MAR/HER	EX	513-693	3.89(13)	0	20436±349	1	2.0
$k_a + k_b$. Pyrolysis in a static system.							
P = (44-282) torr.							
CH_3COO  $\rightarrow \text{CH}_3\text{COOH} +$ 							
Acetic acid cyclohexyl ester (Dicyclohexyl acetate)							
$\rightarrow$ Acetic acid + Cyclohexene							
72 TIN/KOO	EX	613-688	3.16(13)	0	23553±503	1	2.0
Thermolysis.							
 $\rightarrow \text{CH}_3\text{CH}_2\text{OCH}=\text{C}(\text{CH}_3)_2 + \text{CH}_2=\text{C}=\text{O}$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{OCH}=\text{CH}_2 + (\text{CH}_3)_2\text{C}=\text{C}=\text{O}$ (b)							
Cyclobutanone, 3-ethoxy-2,2-dimethyl-							
73 EGG2 ¹⁾	EX	464-558	3.80(13)	0	20267±342	1	1.95
$k_a + k_b$. Based on internal standard technique.							
73 EGG2 ¹⁾	EX	464-558	4.07(13)	0	20292±257	1	1.66
$k_a + k_b$. Based on measurement of amounts of the ethers formed.							
¹⁾ Thermolysis in a static system. P-independent for: $P_0 = (5-50)$ torr. and $P(\text{Total}) < 700$ torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\begin{array}{c} \text{CH}_3 \\ \diagup \\ \text{C} - \text{COOH} \\ \diagdown \\ \text{CH}_3 \end{array} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{C}(\text{CH}_3)_2 + \text{CO}_2$ Cyclopropaneacetic acid, $\alpha, \alpha, 1$-trimethyl- → 2-Pentene, 2,3-dimethyl-, + Carbon dioxide 79 BIG/FET ¹⁾ EX 725 (2.63±0.15)(-2) 1 79 BIG/FET ¹⁾ EX 690-740 (3.32±0.21)(11) 0 21871±505 1 A and B recalculated from the reported data. ¹⁾ Pyrolysis in a Flow-reactor with sealed tubes.							
$\begin{array}{c} \text{CH}_3 \\ \diagup \\ \text{H}_3\text{C} - \text{C} - \text{COOCH}_2\text{CH}_3 \\ \diagdown \\ \text{CH}_3 \end{array} \rightarrow \begin{array}{c} \text{CH}_3 \\ \diagup \\ \text{H}_3\text{C} - \text{C} - \text{COOCH}_2\text{CH}_3 \\ \diagdown \\ \text{CH}_3 \end{array}$ Cyclopropanecarboxylic acid, 2,3-dimethyl-, ethyl ester, (1α, 2α, 3α)- → Cyclopropanecarboxylic acid, 2,3-dimethyl-, ethyl ester, (1α, 2α, 3β)- 77 GAJ/WEB EX 503-548 7.24(11) 0 20081±352 1 Thermal isomerization in a static reactor.							
$\begin{array}{c} \text{CH}_3 \\ \diagup \\ \text{H}_3\text{C} - \text{C} - \text{COOCH}_2\text{CH}_3 \\ \diagdown \\ \text{CH}_3 \end{array} \rightarrow \begin{array}{c} \text{CH}_3 \\ \diagup \\ \text{H}_3\text{C} - \text{C} - \text{COOCH}_2\text{CH}_3 \\ \diagdown \\ \text{CH}_3 \end{array}$ Cyclopropanecarboxylic acid, 2,3-dimethyl-, ethyl ester, (1α, 2α, 3β)- → Cyclopropanecarboxylic acid, 2,3-dimethyl-, ethyl ester, (1α, 2α, 3α)- 77 GAJ/WEB EX 503-548 7.24(11) 0 21540±352 1 Thermal isomerization in a static reactor.							
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{CH}_2\text{C}(\text{O})\text{CH}_3$ → $\text{CH}_3\text{COOH} + \text{CH}_3\text{C}(\text{O})\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ (a) → $\text{CH}_3\text{COOH} + (\text{CH}_3)_2\text{C}=\text{CHC}(\text{O})\text{CH}_3$ (b) 2-Pentanone, 4-(acetyloxy)-4-methyl- 72 TIN/KOO EX 498-563 2.00(12) 0 19326±755 1 3.98 k_a. Thermolysis. 72 TIN/KOO EX 498-563 1.58(11) 0 16205±503 1 2.51 k_b. Thermolysis.							
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$ → $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$ Pentanoic acid 1-methylethyl ester 77 SMI/MUT EX 651 (5.97±0.07)(-3) 1							

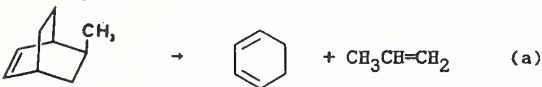
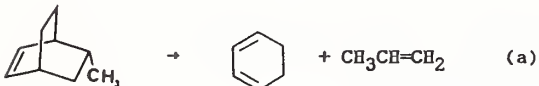
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{C}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHC}(\text{CH}_3)_3$ 1-Butanol, 3,3-dimethyl-, acetate						
79 CHU/MAR Pyrolysis in a static system. P = (63-250) torr.	EX	633-693	2.19(12)	0	23347±505	1 2.24
79 TAY Pyrolysis in a stainless-steel reactor.	EX	660-712	2.24(12)	0	23352	1
$\text{CH}_3\text{C}(\text{O})\text{OCH}(\text{CH}_3)\text{C}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{COOH} + (\text{CH}_3)_3\text{CCH}=\text{CH}_2$ 2-Butanol, 3,3-dimethyl-, acetate						
72 CHU/MAR Static system pyrolysis. P = (25-300) torr.	EX	578-653	3.16(12)	0	22174±302	1 1.66
$(\text{CH}_3)_2\text{CHCH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$ Butanoic acid, 3-methyl-, 1-methylethyl ester						
78 CHU/MAR ¹⁾	EX	603	3.95(-4)			1
78 CHU/MAR ¹⁾	EX	599-629	1.02(13)	0	22798±201	1 1.35
¹⁾ Pyrolysis in a static system. Gas-chromatography.						
$(\text{CH}_3)_3\text{CC}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_3\text{CCOOH} + \text{CH}_3\text{CH}=\text{CH}_2$ Propanoic acid, 2,2-dimethyl-, 1-methylethyl ester						
77 SMI/MUT	EX	651	(7.68±0.32)(-3)			1
78 TAY Pyrolysis.	EX	609-667	1.07(13)	0	22562	1
$\text{CH}_3\text{OCOO}(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{CH}_3\text{OH} + \text{CO}_2 + \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ Carbonic acid hexyl methyl ester						
72 BIG/WRE3	EX	629	1.13			1
72 BIG/WRE3 Flow-tube method. Assumed T-range, omitted in text. The A-factor recalculated from the reported experimental data.	EX	593-648	7.91(15)	0	22949	1
$\text{CH}_3\text{OC}(\text{O})\text{OCH}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ → $\text{CH}_3\text{OH} + \text{CO}_2 + \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (a) → $\text{CH}_3\text{OH} + \text{CO}_2 + \text{cis-CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3$ (b) → $\text{CH}_3\text{OH} + \text{CO}_2 + \text{trans-CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3$ (c) Carbonic acid methyl 1-methylpentyl ester						
72 BIG/WRE3	EX	629	3.53(-2)			1

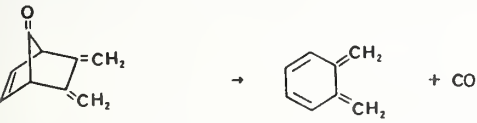
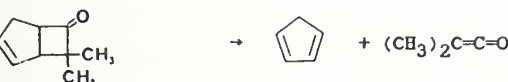
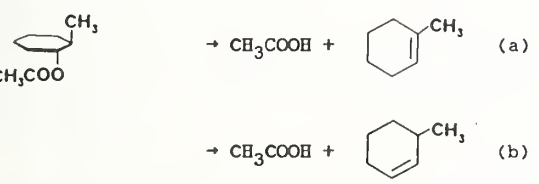
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
72 BIG/WRE3 $k_a + k_b + k_c$. Flow-tube method. Assumed T-range, omitted in text. The A-factor recalculated from the reported experimental data.	EX	598-648	1.91(13)	0	21339	1
$(CH_3)_3C(O)OC(CH_3)_3$						
$\rightarrow (CH_3)_3CO + (CH_3)_3CO$ (a)						
$\rightarrow (CH_3)_2CO + (CH_3)_2CO + CH_3 + CH_3$ (b)						
Peroxide, bis(1,1-dimethylethyl)-						
71 CAD/TRO k_a .	EX	373-423	7.94(14)	0	17922±890	1 9.33
79 SEL/WAD k_a . Thermolysis in a static system.	EX	410	(5.30±0.04)(-5)			1
80 KNO/RIC k_a . Thermolysis of Azomethane and di-t-Butyl peroxide. Mass-spectrometry.	EX	413	(8.9±1.0)(-5)			1
81 ALA/SEL k_a . Thermolysis in a Pyrex vessel. Static system. Mass-spectrometry.	EX	399-434	7.94(15)	0	19246±349	1 2.0
73 PER/GOL k_p . Limiting high-pressure k. RRKM data-fit.	EX	500-660	3.98(15)	0	18822±503	1
$(CH_3)_3CSC(CH_3)_3 \rightarrow$ products						
Propane, 2,2'-thiobis[2-methyl- (di-t-Butyl sulfide)]						
80 MAR/BAR Uninhibited pyrolysis in a static reactor. The products are: Isobutene, Hydrogen sulfide, Isobutane and t-Butylthiol. P = (26-206) torr.	EX	633-686	1.26(15)	0	27545±962	1
$(CH_3)_2CCH_2N=NCH_2CH(CH_3)_2 \rightarrow$ products						
Diazene, bis(2-methylpropyl)-						
78 MCK/TUR 1,1'-Azoisobutane pyrolysis.	EX	553-602	9.12(15)	0	25043±265	1 1.58
$(CH_3)_3CN=NC(CH_3)_3 \rightarrow (CH_3)_3C + (CH_3)_3C + N_2$						
Diazene, bis(1,1-dimethylethyl)-						
73 PER/BEA RRKM fit of experimental data.	EX	503-730	2.51(16)	0	21540±503	1
77 MAR/MAC ¹⁾	EX	483-533	3.98(15)	0	20448±361	1 2.0
77 MCK/TUR ¹⁾	EX	471-531	8.71(15)	0	21086±355	1 2.09

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
 1H-Indene, 2,3,4,7-tetrahydro- → 1H-Indene, 2,3-dihydro- + Hydrogen molecule 72 COC/FRE Pyrolysis in a static system. $P_0 < 0.8$ torr.						
	EX	619-681	8.91(12)	0	24449±237	1 1.45
 Bicyclo[2.2.2]oct-2-ene, 5-methyl-, (1α,4α,5α)- (exo form) → 1,3-Cyclohexadiene + 1-Propene (a) → 1,3-Cyclohexadiene, 5-methyl-, + Ethene (b)						
75 HUY/NGO ¹⁾ k _a .	EX	608-679	5.37(14)	0	29265±40	1 1.07
75 HUY/NGO ¹⁾ k _b .	EX	608-679	1.20(15)	0	29774±40	1 1.07
¹⁾ Pyrolysis in a cylindrical Pyrex vessel. Gas-chromatography. $P = (7-37)$ torr.						
 Bicyclo[2.2.2]oct-2-ene, 5-methyl-, (1α,4α,5β)- (endo form) → 1,3-Cyclohexadiene + 1-Propene (a) → 1,3-Cyclohexadiene, 5-methyl-, + Ethene (b)						
75 HUY/NGO ¹⁾ k _a .	EX	608-679	1.74(14)	0	28163±30	1 1.05
75 HUY/NGO ¹⁾ k _b .	EX	608-679	1.20(14)	0	28138±40	1 1.07
¹⁾ Pyrolysis in a cylindrical Pyrex vessel. Gas-chromatography. $P = (7-37)$ torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
 Bicyclo[2.2.1]hept-2-en-7-one, 5,6-bis(methylene)- (o-Quinodimethane) → 1,3-Cyclohexadiene, 5,6-bis(methylene)- + Carbon monoxide	EX	556-638	(3.1±2.9)(13)	0	12884±554	1
81 ROT/SCH M = N ₂ , or He. Thermolysis. Incident shock-waves. [o-Quinodimethane] = 0.05% (He, N ₂)						
 Bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, (1α,2β,4α)- (endo form) → 1,3-Cyclohexadiene + 2-Propenal (Acrolein)	EX	565-638	9.55(12)	0	23347±55	1 1.10
76 HUY/PAT Retro-Diels-Alder decomposition in a Pyrex vessel. Gas-chromatography. P = (55-240) torr.						
 Bicyclo[3.2.0]hept-2-en-6-one, 7,7-dimethyl- → 1,3-Cyclopentadiene + 1-Propanone, 2-methyl-	EX	470-550	7.94(12)	0	18978±262	1 1.66
73 EGG1 Thermolysis in a static system. Gas-chromatography. P ₀ = (7-68) torr.						
 Cyclohexanol, 2-methyl-acetate, (1R-trans)- → Acetic acid + Cyclohexene, 1-methyl- (a) → Acetic acid + Cyclohexene, 3-methyl- (b)	EX	623-688	2.51(13)	0	23553±503	1 2.51
72 TIN/KOO ¹⁾ k _a + k _b .	EX	623-688	2.51(13)	0	23553±503	1 2.51
72 TIN/KOO ¹⁾ k _a /k _b .	RL	637	1.2			1/1
¹⁾ Thermolysis.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
<chem>CC(=O)OC1CCCCC1</chem> $\rightarrow \text{CH}_3\text{COOH} + \text{Cyclohexene, 1-methyl-}$ (a)							
$\rightarrow \text{CH}_3\text{COOH} + \text{Cyclohexene, 3-methyl-}$ (b)							
Cyclohexanol, 2-methyl-acetate, (1S-cis)-							
$\rightarrow$ Acetic acid + Cyclohexene, 1-methyl- (a)							
$\rightarrow$ Acetic acid + Cyclohexene, 3-methyl- (b)							
72 TIN/KOO ¹⁾	EX	623-688	6.31(13)	0	24157±503	1	3.98
$k_a + k_b$.							
72 TIN/KOO ¹⁾	RL	637	8.6(-1)			1/1	
k_b/k_a .							
¹⁾ Thermolysis.							
<chem>CC(=O)OC(C)CC(C)C</chem>							
$\rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}(\text{CH}_3)_2$ (a)							
$\rightarrow \text{CH}_3\text{COOH} + \text{cis}-(\text{CH}_3)_2\text{C}=\text{CHCH}(\text{CH}_3)_2$ (b)							
$\rightarrow \text{CH}_3\text{COOH} + \text{trans}-(\text{CH}_3)_2\text{C}=\text{CHCH}(\text{CH}_3)_2$ (c)							
2-Pentanol, 2,4-dimethyl-, acetate							
79 TAY	RL	673	1.85			1/1	
$k_a/(k_b + k_c)$. Pyrolysis in a stainless-steel reactor. Gas-chromatography. The % of alkene-1 and alkene-2 reported in the text (61.5 and 38.5 respectively) give a ratio of only 1.60.							
<chem>CC(=O)OC(C)CC(C)(C)C</chem>							
$\rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{C}(\text{CH}_3)_3$ (a)							
$\rightarrow \text{CH}_3\text{COOH} + \text{cis-CH}_3\text{CH}=\text{CHC}(\text{CH}_3)_3$ (b)							
$\rightarrow \text{CH}_3\text{COOH} + \text{trans-CH}_3\text{CH}=\text{CHC}(\text{CH}_3)_3$ (c)							
2-Pentanol, 4,4-dimethyl-, acetate							
79 TAY	RL	668-778	4.9(-1)			1/1	
$k_a/(k_b + k_c)$. Pyrolysis in a stainless-steel reactor. Gas-chromatography.							
81 CHU/DOM	EX	573-623	7.41(14)	0	21796±409	1	2.04
$k_a + k_b + k_c$. Pyrolysis in a static system.							
NMR-spectroscopy. P = (48-211) torr.							
<chem>CC(=O)OC(C)CC(C)C</chem> $\rightarrow \text{CH}_3\text{COOH} + (\text{CH}_3)_3\text{CCH}=\text{CHCH}_3$							
3-Pentanol, 2,2-dimethyl-, acetate							
72 CHU/MAR	EX	578-653	1.15(13)	0	22572±393	1	1.23
Pyrolysis in a static system.							
P = (25-300) torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

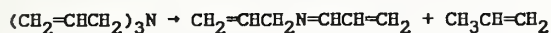
Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{C}(\text{O})\text{OC}[\text{CH}(\text{CH}_3)_2](\text{CH}_3)\text{CH}_2\text{CH}_3$ $\rightarrow \text{CH}_3\text{COOH} + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_3\text{COOH} + \text{cis-CH}_3\text{CH}=\text{C}[\text{CH}(\text{CH}_3)_2]\text{CH}_3$ (b) $\rightarrow \text{CH}_3\text{COOH} + \text{trans-CH}_3\text{CH}=\text{C}[\text{CH}(\text{CH}_3)_2]\text{CH}_3$ (c)							
3-Pentanol, 2,3-dimethyl-, acetate							
77 CUE/CHU $k_a + k_b + k_c$	EX	485-533	1.66(14)	0	20433±252	1	1.69
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{C}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)_3$ 2-Butanol, 2,3,3-trimethyl-, acetate							
80 MAR/CHU Pyrolysis. Static system. P = (56-210) torr.	EX	503-513	2.51(14)	0	20629±553	1	3.09
$(\text{CH}_3)_3\text{CC}(\text{O})\text{OC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_3\text{COOH} + (\text{CH}_3)_2\text{C}=\text{CH}_2$ Propanoic acid, 2,2-dimethyl-, 1,1-dimethylethyl ester							
78 TAY Pyrolysis.	EX	519-608	1.05(13)	0	19884	1	
$(\text{CH}_3\text{CH}_2)_2\text{CHC}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3\text{CH}_2)_2\text{CHCOOH} + \text{CH}_3\text{CH}=\text{CH}_2$ Butanoic acid, 2-ethyl-, 1-methylethyl ester							
77 SMI/MUT	EX	651	(6.97±0.17)(-3)			1	
$(\text{CH}_3)_3\text{CCH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_3\text{CCH}_2\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$ Butanoic acid, 3,3-dimethyl-, 1-methylethyl ester							
77 SMI/MUT	EX	651	(5.95±0.19)(-3)			1	
78 CHU/MAR Pyrolysis in a static system.	EX	589-628	4.47(13)	0	23704±324	1	1.74
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$ Pentanoic acid, 2-methyl-, 1-methylethyl ester							
77 SMI/MUT	EX	651	(6.88±0.24)(-3)			1	
$\text{CH}_3(\text{CH}_2)_4\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$ Hexanoic acid 1-methylethyl ester							
77 SMI/MUT	EX	651	(6.03±0.27)(-3)			1	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OC}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CO}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$ Carbonic acid dibutyl ester (Di-n-butyl carbonate)							
72 BIG/WRE1 ¹) Sealed-tube pyrolysis.	EX	554-594	1.32(12)	0	21892	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
72 BIG/WRE1 ¹⁾	EX	700	(9.70±0.29)(-2)			1
72 BIG/WRE1 ¹⁾ Flow-tube pyrolysis. The A-factor recalculated from the reported data.	EX	563-708	(1.56±0.05)(13)	0	22899	1
¹⁾ Pyrolysis in Kooyman, or break-seal tubes.						
$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{OC}(\text{O})\text{OCH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CO}_2 + \text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{CH}_3$ (a) $\rightarrow \text{cis-CH}_3\text{CH}=\text{CHCH}_3 + \text{CO}_2 + \text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{CH}_3$ (b) $\rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}_3 + \text{CO}_2 + \text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{CH}_3$ (c)						
Carbonic acid bis(1-methylpropyl) ester (Di-s-butyl carbonate)						
72 BIG/WRE2 ¹⁾ Flow-tube pyrolysis.	EX	629	5.25(-2)			1
72 BIG/WRE2 ¹⁾ Flow-tube pyrolysis. The A-factor recalculated from the reported data.	EX	593-648	1.50(13)	0	20936	1
72 BIG/WRE2 ¹⁾ Sealed-tube pyrolysis.	EX	629	6.09(-2)			1
72 BIG/WRE2 ¹⁾ Sealed-tube pyrolysis.	EX	489-540	9.07(12)	0	20533	1
¹⁾ Pyrolysis in Kooyman, or break-seal tubes.						
$(\text{CH}_3)_2\text{CHCH}_2\text{OC}(\text{O})\text{OCH}_2\text{CH}(\text{CH}_3)_2$ $\rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CO}_2 + (\text{CH}_3)_2\text{CHCH}_2\text{OH}$						
Carbonic acid bis(2-methylpropyl) ester (Di-i-butyl carbonate)						
72 BIG/WRE1 ¹⁾	EX	700	3.2(-1)			1
72 BIG/WRE1 ¹⁾ The A-factor recalculated from the reported data.	EX	563-708	(5.53±0.17)(13)	0	24560	1
¹⁾ Pyrolysis in the Kooyman flow-tube.						
$(\text{CH}_3)_3\text{COC}(\text{O})\text{OC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_3\text{COH} + \text{CO}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2$						
Carbonic acid bis(1,1-dimethylethyl) ester (Di-t-butyl carbonate)						
72 BIG/WRE3 Sealed-tube.	EX	453-498	2.4(13)	0	19124	1
72 BIG/WRE3	EX	629	2.01			1
72 BIG/WRE3 Flow-tube. Assumed T-range, omitted in text. A-factor recalculated from the reported data.	EX	593-648	1.31(12)	0	17111	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
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2-Propen-1-amine, N,N-di-2-propenyl- (Triallylamine)

→ 2-Propen-1-amine, N-2-propenylidene- + 1-Propene

74 VIT/EGG1 EX 531-620 5.50(11) 0 19260±96 1 1.17

Thermolysis.

Static system.

N-2-Propenylidene-2-propen-1-amine undergoes cyclization to give 3-Methylpyridine.

P(Triallylamine) = (3-36) torr.

P(Total) = (23-178) torr.



Cyclohexanamine, N-2-propenyl-

→ 1-Propene + Cyclohexanimine

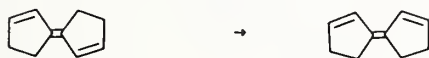
73 EGG3 EX 562-652 2.75(11) 0 21228±287 1 1.62

Thermolysis in a static system.

Gas-chromatography.

k is P-independent within the given P-range.

P = (15-150) torr.



Cyclopentene, 3-(cyclopent-4-en-1-ylidene)-

(trans form)

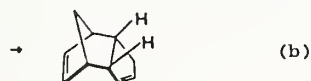
→ Cyclopentene, 3-(cyclopent-2-en-1-ylidene)-

(cis form)

73 DOE/BEA EX 526-576 1.07(12) 0 20986±403 1 2.09

Thermal isomerization in a 12 l. Pyrex flask,

or in a 3.5 l. Corning lead-potash flask.



Tricyclo[5.3.0.0^{2,6}]deca-3,9-diene

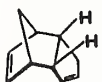
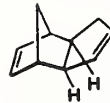
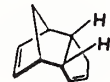
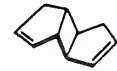
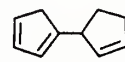
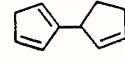
(anti-cis-[2+2]-Dicyclopentadiene)

→ 1,3-Cyclopentadiene + 1,3-Cyclopentadiene (a)

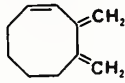
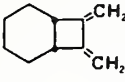
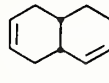
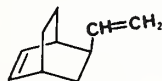
→ Tricyclo[5.2.1.0^{2,6}]deca-3,8-diene, endo-

(endo-[2+4]-Dicyclopentadiene) (b)

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 $\rightarrow$  $+$  Tricyclo[5.2.1.0 ^{2,6}]deca-3,8-diene, endo- (endo-[2+4]-Dicyclopentadiene) $\rightarrow$ 1,3-Cyclopentadiene + 1,3-Cyclopentadiene	EX	431-494	(2.0 $\pm$ 0.4)(14)	0	18671 $\pm$ 101	1	
81 GRI/SCH Thermolysis. P = (2-3) torr.							
 $\rightarrow$  $+$  Tricyclo[5.2.1.0 ^{2,6}]deca-3,8-diene, exo- (exo-[2+4]-Dicyclopentadiene) $\rightarrow$ 1,3-Cyclopentadiene + 1,3-Cyclopentadiene	EX	481-551	(5.6 $\pm$ 0.4)(14)	0	21389 $\pm$ 50	1	
81 GRI/SCH Thermolysis. P = (2-3) torr.							
 $\rightarrow$  $+$  (a)							
$\rightarrow$  (b)							
$\rightarrow$  (c)							
$\rightarrow$  (d)							
$\rightarrow$  (e)							
Tricyclo[4.2.1.1 ^{2,5}]deca-3,7-diene, (1 α ,2 β ,5 β ,6 α)- (anti-[4+4]-Dicyclopentadiene) $\rightarrow$ 1,3-Cyclopentadiene + 1,3-Cyclopentadiene (a) $\rightarrow$ Tricyclo[5.2.1.0 ^{2,6}]deca-3,8-diene, endo- (b) $\rightarrow$ Tricyclo[5.3.0.0 ^{2,6}]deca-3,9-diene (c) $\rightarrow$ 1,3-Cyclopentadiene, 1-(2-cyclopenten-1-yl)- (d) $\rightarrow$ 1,3-Cyclopentadiene, 2-(2-cyclopenten-1-yl)- (e)	EX	460-532	(5.0 $\pm$ 0.9)(14)	0	20030 $\pm$ 101	1	
81 GRI/SCH k _{overall} . Thermolysis. P = (2-3) torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

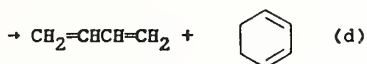
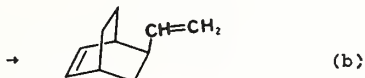
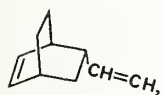
Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2=\text{C}=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{C}=\text{CH}_2 \rightarrow$  (a)						
$\rightarrow$  (b)						
1,2,8,9-Decatetraene						
→ Cyclooctene, 3,4-bis(methylene)- (a)						
→ Bicyclo[4.2.0]octane, 7,8-bis(methylene)-, cis- (b)						
82 GAJ/BEN	EX	633-693	2.5(9)	0	15501	1
$k_a + k_b$. Pyrolysis.						
Flow-system. Intramolecular Allene addition.						
Major product given by (a).						
 $\rightarrow$  (a)						
$\rightarrow$  (b)						
$\rightarrow$  (c)						
$\rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 +$  (d)						
Bicyclo[4.2.2]deca-3,7-diene						
→ Naphthalene, 1,2,4a,5,8,8a-hexahydro-, cis- (a)						
→ Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-, (1 α ,4 α ,5 α)- (exo form) (b)						
→ Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-, (1 α ,4 α ,5 β)- (endo form) (c)						
→ 1,3-Butadiene + 1,3-Cyclohexadiene (d)						
82 HUY/HUB1 ¹)	EX	456-526	4.37(14)	0	22662±35	1 1.07
k_a . Thermal isomerization.						
82 HUY/HUB1 ¹)	EX	456-526	4.17(14)	0	23437±35	1 1.07
k_b . Thermal isomerization.						
82 HUY/HUB1 ¹)	EX	456-526	1.41(14)	0	23342±45	1 1.10
k_c . Thermal isomerization.						
82 HUY/HUB1 ¹)	EX	456-526	5.25(15)	0	24826±35	1 1.07
k_d . Thermolysis.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
1) Thermal isomerization, or decomposition in a static system with cylindrical packed, or unpacked Pyrex vessels. Gas-chromatography. NMR-, IR-, and Mass-spectrometry. $P_0 = (2-40)$ torr.							
	→						(a)
	→						(b)
	→						(c)
	→		$\text{CH}_2=\text{CHCH}=\text{CH}_2 + $				(d)
Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-, (1α,4α,5α)- (exo form)							
→ Naphthalene, 1,2,4a,5,8,8a-hexahydro-, cis-							(a)
→ Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-, (1α,4α,5β)- (endo form)							(b)
→ Bicyclo[4.2.2]deca-3,7-diene							(c)
→ 1,3-Butadiene + 1,3-Cyclohexadiene							(d)
82 HUY/HUB1 1) k_a . Thermal isomerization.	EX	513-578	1.05(14)	0	25450±91	1	1.17
82 HUY/HUB1 1) k_b . Thermal isomerization.	EX	513-578	9.33(13)	0	25798±101	1	1.20
82 HUY/HUB1 1) k_c . Thermal isomerization.	EX	513-578	2.57(13)	0	24731±161	1	1.35
82 HUY/HUB1 1) k_a . Thermolysis. Calculated by combining several k's measured in this work with their respective equilibrium constants.	DE	513-578	8.91(14)	0	26694±50	1	1.10
1) Thermal isomerization, or decomposition in a static system with cylindrical packed, or unpacked Pyrex vessels. Gas-chromatography. NMR-, IR-, and Mass-spectrometry. $P_0 = (2-40)$ torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/(ref), A, A/(ref)	n	B, B-B(ref)	k, A k err. units factor
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Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-, (1α,4α,5β)-
(endo form)

→ Naphthalene, 1,2,4a,5,8,8a-hexahydro, cis- (a)

→ Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-,
(1α,4α,5α)- (exo form) (b)

→ Bicyclo[4.2.2]deca-3,7-diene (c)

→ 1,3-Butadiene + 1,3-Cyclohexadiene (d)

82 HUY/HUB1 ¹⁾ EX 476-563 8.91(12) 0 22416±60 1 1.12

k_a . Thermal isomerization.

82 HUY/HUB1 ¹⁾ DE 476-563 8.91(13) 0 25949±292 1 1.70

k_b . Thermal isomerization. Calculated by
combining several k 's measured in this work
with their respective equilibrium constants.

82 HUY/HUB1 ¹⁾ DE 476-563 8.13(12) 0 24791±232 1 1.51

k_c . Thermal isomerization. Calculated by
combining several k 's measured in this work
with their respective equilibrium constants.

82 HUY/HUB1 ¹⁾ EX 476-563 2.88(14) 0 25908±101 1 1.20

k_d . Thermolysis.

¹⁾ Thermolysis in a static system with cylindrical
packed, or unpacked Pyrex vessels.

Gas-chromatography. $P_0 = (2-40)$ torr.

$\text{CH}_3(\text{CH}_2)_8\text{CH}_3 \rightarrow \text{products}$

Decane

71 GON/LEW EX 713-793 1.95(3) 0 13337 1

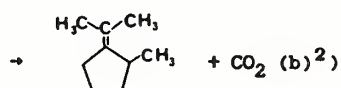
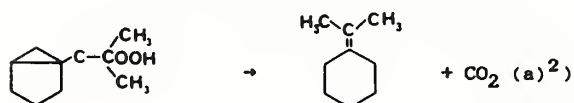
80 RUM/SHE EX 918-958 2.19(14) 0 31274±4126 1 11.22

Pyrolysis in a quartz reactor.

$P = 760$ torr.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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Bicyclo[3.1.0]hexane-1-acetic acid, α, α -dimethyl-

→ Cyclohexane, (1-methylethylidene)-

+ Carbon dioxide (a)

→ Cyclopentane, 1-methyl-2-(1-methylethylidene)-

+ Carbon dioxide (b)

79 BIG/FET ¹⁾ k_a .	EX	725 ^a	1.56(-2)			1
79 BIG/FET ¹⁾ k_b .	EX	725	9.7(3)			1
79 BIG/FET ¹⁾ $k_a + k_b$.	EX	725	(2.53±0.10)(-2)			1
79 BIG/FET ¹⁾ $k_a + k_b$.	EX	690-740	(9.21±0.36)(10)	0	20969±806	1

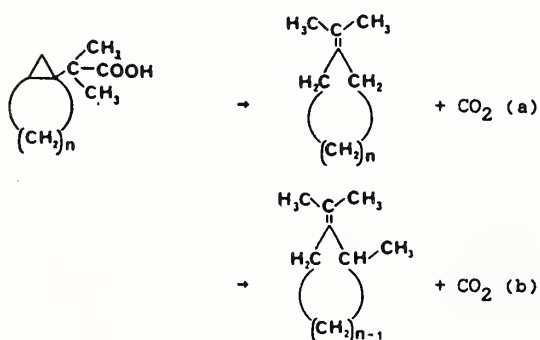
A and B recalculated from the reported experimental data.

1) Pyrolysis in a Flow-reactor with evacuated sealed tubes.

Gas-chromatography.

NMR-spectroscopy.

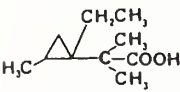
2) The general mechanism of this type of reaction is:



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

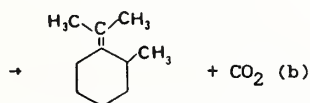
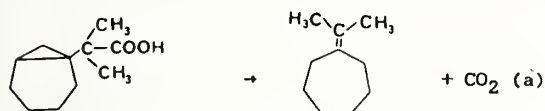
Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH_3COO  $\rightarrow \text{CH}_3\text{COOH} +$  (a)							
$\rightarrow \text{CH}_3\text{COOH} +$  (b)							
1,2-Cyclohexanediol diacetate, trans-							
→ Acetic acid + 1-Cyclohexen-1-ol acetate (a)							
→ Acetic acid + 2-Cyclohexen-1-ol acetate (b)							
72 TIN/KOO ¹⁾	EX	643-733	3.16(12)	0	24006±503	1	2.0
$k_a + k_b$.							
72 TIN/KOO ¹⁾	RL	637	4.0(-1)			1/1	
k_a/k_b .							
¹⁾ Thermolysis.							
CH_3COO  $\rightarrow \text{CH}_3\text{COOH} +$  (a)							
$\rightarrow \text{CH}_3\text{COOH} +$  (b)							
1,2-Cyclohexanediol diacetate, cis-							
→ Acetic acid + 1-Cyclohexen-1-ol acetate (a)							
→ Acetic acid + 2-Cyclohexen-1-ol acetate (b)							
72 TIN/KOO ¹⁾	EX	643-733	5.01(12)	0	24157±1510	1	3.16
$k_a + k_b$.							
72 TIN/KOO ¹⁾	RL	637	1.46(-1)			1/1	
k_b/k_a .							
¹⁾ Thermolysis.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}[\text{C}(\text{CH}_3)_3]\text{CH}_2\text{CH}=\text{CH}_2$							
→ $\text{CH}_3\text{COOH} + \text{cis}-(\text{CH}_3)_3\text{CCH}=\text{CHCH}=\text{CH}_2$ (a)							
→ $\text{CH}_3\text{COOH} + \text{trans}-(\text{CH}_3)_3\text{CCH}=\text{CHCH}=\text{CH}_2$ (b)							
5-Hexen-3-ol, 2,2-dimethyl-, acetate							
→ 1,3-Hexadiene, 5,5-dimethyl-, (Z)- (a)							
→ 1,3-Hexadiene, 5,5-dimethyl-, (E)- (b)							
73 CHU/PIO	EX	573-623	1.38(14)	0	23352±302	1	1.02
$k_a + k_b$.							
Pyrolysis in a static system.							
P = (35-300) torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 $\rightarrow (\text{CH}_3)_2\text{CHC}(\text{CH}_2\text{CH}_3)=\text{C}(\text{CH}_3)_2 + \text{CO}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_2\text{CH}_3)=\text{C}(\text{CH}_3)_2 + \text{CO}_2$ (b) Cyclopropaneacetic acid, 1-ethyl- α,α ,2-trimethyl- $\rightarrow$ 2-Pentene, 3-ethyl-2,4-dimethyl- + Carbon dioxide (a) $\rightarrow$ 2-Hexene, 3-ethyl-2-methyl- + Carbon dioxide (b)							
79 BIG/FET ¹⁾ $k_a = k_b$.	EX	725	5.25(-3)				1
79 BIG/FET ¹⁾ $k_a + k_b$.	EX	725	(1.05 $\pm$ 0.10)(-2)				1
79 BIG/FET ¹⁾ $k_a + k_b$. A and B recalculated from the reported data.	EX	690-740	(1.41 $\pm$ 0.13)(11)	0	21919 $\pm$ 625		1
¹⁾ Pyrolysis in a Flow-reactor with evacuated sealed tubes. Gas-chromatography. NMR-spectroscopy.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}[\text{CH}(\text{CH}_3)_2]\text{C}(\text{CH}_3)_3$ $\rightarrow \text{CH}_3\text{COOH} + (\text{CH}_3)_3\text{CCH}=\text{C}(\text{CH}_3)_2$ 3-Pentanol, 2,2,4-trimethyl-, acetate							
72 CHU/MAR Pyrolysis in a static system. P = (25-300) torr.	EX	578-653	1.32(13)	0	23452 $\pm$ 116	1	1.20
$(\text{CH}_3)_3\text{CCH}_2\text{C}(\text{O})\text{OC}(\text{CH}_3)_3$ $\rightarrow (\text{CH}_3)_3\text{CCH}_2\text{COOH} + (\text{CH}_3)_2\text{C}=\text{CH}_2$ Butanoic acid, 3,3-dimethyl-, 1,1-dimethylethyl ester							
78 TAY Pyrolysis.	EX	558-620	5.24(12)	0	19527	1	
 $\rightarrow$  + $\text{CH}_3\text{CH}=\text{CH}_2$							
Benzene, [(2-propenylthio)methyl]- (Allyl benzyl sulfide) $\rightarrow$ Benzenecarbothioaldehyde + 1-Propene							
82 MAR/ROP2 Pyrolysis. Stirred-flow. Benzene carbothio- aldehyde [Benzylthioaldehyde] polymerizes into into an amorphous solid. P = (2-15) torr.	EX	588-691	8.51(10)	0	16960 $\pm$ 241	1	1.51

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
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Bicyclo[4.1.0]heptane-1-acetic acid, α, α -dimethyl-

→ Cycloheptane, (1-methylethylidene)-

+ Carbon dioxide (a)

→ Cyclohexane, 1-methyl-2-(1-methylethylidene)-

+ Carbon dioxide (b)

79 BIG/FET ¹⁾ EX 725 3.09(-2) 1

k_a .

79 BIG/FET ¹⁾ EX 725 8.7(-3) 1

k_b .

79 BIG/FET ¹⁾ EX 725 (3.96±0.16)(-2) 1

$k_a + k_b$.

79 BIG/FET ¹⁾ EX 690-740 (6.81±0.28)(9) 0 18756±854 1

$k_a + k_b$.

A and B recalculated from the reported data.

¹⁾ Pyrolysis in a Flow-reactor with evacuated sealed

tubes. Gas-chromatography. NMR-spectroscopy.

See footnote ²⁾ above for the general mechanism

of this type of reaction.



endo-Tricyclo[6.2.2.0^{2,7}]dodeca-3,9-diene

→ 1,3-Cyclohexadiene + 1,3-Cyclohexadiene

71 DEM/HUY EX 471-739 2.51(14) 0 26170±956 1 5.01

Thermolysis in a Pyrex vessel.

P = (4-20) torr.

CH3(CH2)10CH3 → products

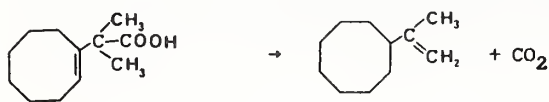
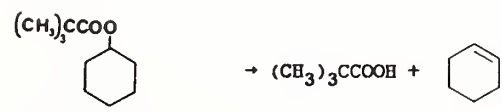
Dodecane

80 RUM/SHE EX 873-953 8.91(13) 0 30216±1010 1 3.02

Pyrolysis in a quartz reactor.

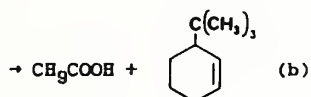
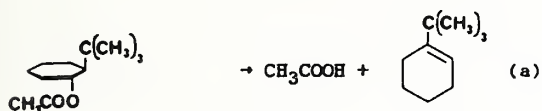
P = 760 torr.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
							
1-Cyclooctene-1-acetic acid, α, α -dimethyl- → Cyclooctane, (1-methylethenyl)- + Carbon dioxide							
77 BIG/WEA 1)	RL	500	1.9				1/1
k/k _{ref} : k _{ref} : CH ₃ CH=C(CH ₂ CH ₃)C(CH ₃) ₂ COOH → CH ₃ CH=C(CH ₃ CH ₃)CH(CH ₃) ₂ + CO ₂							
77 BIG/WEA 1,	EX	500	1.66(-4)				1
1) Pyrolysis in a flow-reactor. Gas-chromatography.							
							
Propanoic acid, 2,2-dimethyl-, cyclohexyl ester (Cyclohexyl pivalate) → Propanoic acid, 2,2-dimethyl- (Pivalic acid) + Cyclohexene							
72 TIN/KOO	EX	613-663	1.0(13)	0	22647±1007	1	5.01
Thermolysis.							
CH ₃ CH ₂ C(CH ₃) ₂ OOC(CH ₃) ₂ CH ₂ CH ₃ → products Peroxide, bis(1,1-dimethylpropyl)-							
73 PER/GOL	EX	523-633	6.31(15)	0	18319±503	1	
A and B factors recommended for T = 300 K. Limiting high-pressure k. RRKM data-fit.							
(CH ₃ CH ₂ CH ₂) ₂ CHC(O)OCH(CH ₃) ₂ → (CH ₃ CH ₂ CH ₂) ₂ CHCOOH + CH ₃ CH=CH ₂							
Pentanoic acid, 2-propyl-, 1-methylethyl ester							
77 SMI/MUT	EX	651	(6.89±0.30)(-3)				1
CH ₃ CH ₂ C(CH ₃) ₂ OC(O)OC(CH ₃) ₂ CH ₂ CH ₃ → CH ₃ CH ₂ C(CH ₃) ₂ OH + CO ₂ + CH ₂ =C(CH ₃)CH ₂ CH ₃ (a) → CH ₃ CH ₂ C(CH ₃) ₂ OH + CO ₂ + (CH ₃) ₂ C=CHCH ₃ (b)							
Carbonic acid bis(1,1-dimethylpropyl) ester							
72 BIG/WRE3	EX	629	4.05				1
72 BIG/WRE3	EX	593-648	1.03(13)	0	17967		1
k _a + k _b . Flow-tube method. Assumed T-range, omitted in text. A and B recalculated from the reported data.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
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Cyclohexanol, 2-(1,1-dimethylethyl)-acetate, trans-

$\rightarrow$ Acetic acid + Cyclohexene,

1-(1,1-dimethylethyl)- (a)

$\rightarrow$ Acetic acid + Cyclohexene,

3-(1,1-dimethylethyl)- (b)

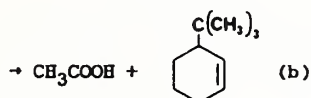
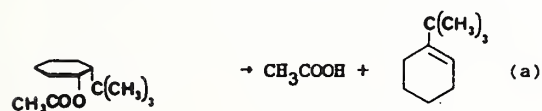
72 TIN/KOO ¹⁾ EX 588-643 6.31(13) 0 22144±1510 1 10.0

$k_a + k_b$.

72 TIN/KOO ¹⁾ RL 637 3.0 1/1

k_a/k_b .

¹⁾ Thermolysis.



Cyclohexanol, 2-(1,1-dimethylethyl)-acetate, cis-

$\rightarrow$ Acetic acid + Cyclohexene,

1-(1,1-dimethylethyl)- (a)

$\rightarrow$ Acetic acid + Cyclohexene,

3-(1,1-dimethylethyl)- (b)

72 TIN/KOO ¹⁾ EX 618-688 1.26(13) 0 23654±1007 1 5.01

$k_a + k_b$.

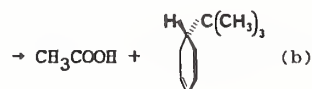
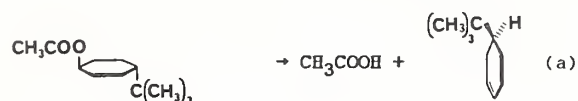
72 TIN/KOO ¹⁾ RL 637 1.20 1/1

k_b/k_a .

¹⁾ Thermolysis.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
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Cyclohexanol, 4-(1,1-dimethylethyl)-acetate, trans-

→ Acetic acid + Cyclohexene,

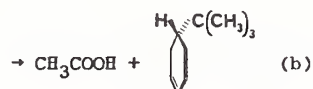
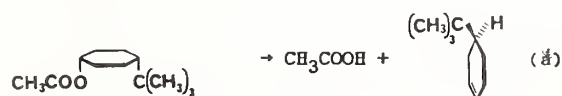
4-(1,1-dimethylethyl)- (R), (a)

→ Acetic acid + Cyclohexene,

4-(1,1-dimethylethyl)- (S), (b)

72 TIN/KOO ¹⁾	EX	618-698	1.26(12)	0	21641±1510	1	10.0
$k_a + k_b$.							

72 TIN/KOO ¹⁾	RL	637	1.0				1/1
k_a/k_b .							

¹⁾ Thermolysis.

Cyclohexanol, 4-(1,1-dimethylethyl)-acetate, cis-

→ Acetic acid + Cyclohexene,

4-(1,1-dimethylethyl)-, (R)- (a)

→ Acetic acid + Cyclohexene,

4-(1,1-dimethylethyl)-, (S)- (b)

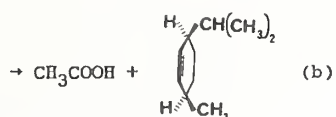
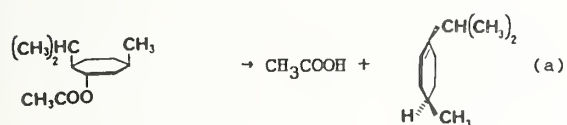
72 TIN/KOO ¹⁾	EX	618-698	3.16(12)	0	21641±1510	1	10.0
$k_a + k_b$.							

72 TIN/KOO ¹⁾	RL	637	1.0				1/1
k_a/k_b .							

¹⁾ Thermolysis.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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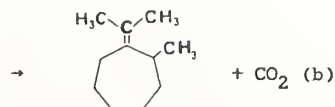
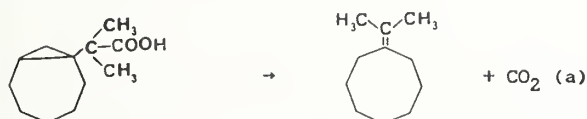
Cyclohexanol, 5-methyl-2-(1-methylethyl)-
 acetate, (1 α , 2 β , 5 β)-
 (trans-2-Isopropyl-1-menthyl acetate)

→ Acetic acid + Cyclohexene, 4-methyl-
 1-(1-methylethyl)- (a)

→ Acetic acid + Cyclohexene, 3-methyl-
 6-(1-methylethyl)-, cis- (b)

72 TIN/KOO ¹⁾ k _a + k _b .	EX	598-673	5.01(12)	0	21943±503	1 2.0
72 TIN/KOO ¹⁾ k _a /k _b .	RL	637	1.8			1/1

¹⁾ Thermolysis. The reactant exists in two forms:
 5 α and 5 β , not specified in the text. Only the
 form 5 β is given here.



Bicyclo[5.1.0]octane-1-acetic acid, α , α -dimethyl-
 → Cyclooctane, (1-methylethylidene)-

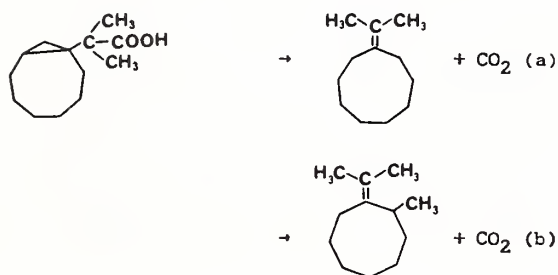
+ Carbon dioxide (a)

→ Cycloheptane, 1-methyl-2-(1-methylethylidene)-
 + Carbon dioxide (b)

79 BIG/FET ¹⁾ k _a .	EX	725	4.56(-2)			1
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4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 BIG/FET ¹⁾ k _b .	EX	725	5.3(-3)			1
79 BIG/FET ¹⁾ k _a + k _b .	EX	725	(5.09±0.21)(-2)			1
79 BIG/FET ¹⁾ k _a + k _b . A and B recalculated from the reported data.	EX	690-740	(3.82±0.16)(9)	0	18154±758	1
¹⁾ Pyrolysis in a Flow-reactor with evacuated sealed tubes. Gas-chromatography. NMR-spectroscopy. See footnote ²⁾ above for the general mechanism of this type of reaction.						

Bicyclo[6.1.0]nonane-1-acetic acid, α, α -dimethyl-

→ Cyclononane, (1-methylethylidene)-

+ Carbon dioxide (a)

→ Cyclooctane, 1-methyl-2-(1-methylethylidene)-

+ Carbon dioxide (b)

79 BIG/FET ¹⁾ k _a .	EX	725	5.67(-2)			1
79 BIG/FET ¹⁾ k _b .	EX	725	4.8(-3)			1
79 BIG/FET ¹⁾ k _a + k _b .	EX	725	(6.15±0.19)(-2)			1
79 BIG/FET ¹⁾ k _a + k _b . A and B recalculated from the reported data.	EX	690-740	(2.95±0.09)(9)	0	17829±1107	1

¹⁾ Pyrolysis in a Flow-reactor with evacuated sealed tubes.
Gas-chromatography.
NMR-spectroscopy.
See footnote ²⁾ above for the general mechanism of this type of reaction.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref)), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3(\text{CH}_2)_5\text{OC}(\text{O})\text{O}(\text{CH}_2)_5\text{CH}_3$ $\rightarrow \text{CH}_3(\text{CH}_2)_5\text{OH} + \text{CO}_2 + \text{CH}_2=\text{CH}(\text{CH}_2)_3\text{CH}_3$ Carbonic acid dihexyl ester (Di-n-hexyl carbonate)						
72 BIG/WRE1 ¹⁾ Sealed-tube pyrolysis.	EX	554-594	4.2(12)	0	22496	1
72 BIG/WRE1 ¹⁾	EX	700	(1.30±0.04)(-1)			1
72 BIG/WRE1 ¹⁾ Flow-tube pyrolysis. The A-factor recalculated from the reported data.	EX	663-708	(7.65±0.23)(12)	0	22194	1
¹⁾ Pyrolysis in Kooyman or break-seal tubes.						
$\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_3)\text{OC}(\text{O})\text{OCH}(\text{CH}_3)(\text{CH}_2)_3\text{CH}_3$ $\rightarrow \text{CH}_3(\text{CH}_2)_3\text{CH}=\text{CH}_2 + \text{CO}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{OH})\text{CH}_3$ (a) $\rightarrow \text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{CO}_2$ $\quad + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{OH})\text{CH}_3$ (b) $\rightarrow \text{trans-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{CO}_2$ $\quad \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{OH})\text{CH}_3$ (c) Carbonic acid bis(1-methylpentyl) ester						
72 BIG/WRE2 $k_a + k_b + k_c$.	EX	629	6.29(-2)			1
72 BIG/WRE2 $k_a + k_b + k_c$. The A-factor recalculated from the reported data.	EX	593-648	6.34(12)	0	20282	1
¹⁾ Flow-tube pyrolysis.						
$\text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{OOCH}_2(\text{CH}_2)_5\text{CH}_3$ $\rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{O} + \text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{O}$ Peroxide, diheptyl-						
82 SAH/RIG Decomposition in a O ₂ /CO ₂ mixture, in a quartz vessel. P(Total) = 180 torr.	EX	509	(6.7±1.4)(-1)			1
$\text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{products}$ Pentadecane						
80 RUM/SHE Pyrolysis in a quartz reactor. P = 760 torr.	EX	888-993	2.95(14)	0	31370±1612	1 6.03

5. References to the Table

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6. Conversion Factors for Rate Constants

Equivalent second order rate constants

A \ B	cm ³ mol ⁻¹ s ⁻¹	dm ³ mol ⁻¹ s ⁻¹	m ³ mol ⁻¹ s ⁻¹	cm ³ molecule ⁻¹ s ⁻¹	(mm Hg) ⁻¹ s ⁻¹	atm ⁻¹ s ⁻¹	ppm ⁻¹ min ⁻¹	m ² kN ⁻¹ s ⁻¹
1 cm ³ mol ⁻¹ s ⁻¹ =	1	10 ⁻³	10 ⁻⁶	1.66 × 10 ⁻²⁴	1.604 × 10 ⁻⁵ T ⁻¹	1.219 × 10 ⁻² T ⁻¹	2.453 × 10 ⁻⁹	1.203 × 10 ⁻⁴ T ⁻¹
1 dm ³ mol ⁻¹ s ⁻¹ =	10 ³	1	10 ⁻³	1.66 × 10 ⁻²¹	1.604 × 10 ⁻² T ⁻¹	12.19 T ⁻¹	2.453 × 10 ⁻⁶	1.203 × 10 ⁻¹ T ⁻¹
1 m ³ mol ⁻¹ s ⁻¹ =	10 ⁶	10 ³	1	1.66 × 10 ⁻¹⁸	16.04 T ⁻¹	1.219 × 10 ⁴ T ⁻¹	2.453 × 10 ⁻³	120.3 T ⁻¹
1 cm ³ molecule ⁻¹ s ⁻¹ =	6.023 × 10 ²³	6.023 × 10 ²⁰	6.023 × 10 ¹⁷	1	9.658 × 10 ¹⁸ T ⁻¹	7.34 × 10 ²¹ T ⁻¹	1.478 × 10 ¹⁵	7.244 × 10 ¹⁹ T ⁻¹
1 (mm Hg) ⁻¹ s ⁻¹ =	6.236 × 10 ⁴ T	62.36 T	6.236 × 10 ⁻² T	1.035 × 10 ⁻¹⁹ T	1	760	4.56 × 10 ⁻²	7.500
1 atm ⁻¹ s ⁻¹	82.06 T	8.206 × 10 ⁻² T	8.206 × 10 ⁻⁵ T	1.362 × 10 ⁻²² T	1.316 × 10 ⁻³	1	6 × 10 ⁻⁵	9.869 × 10 ⁻³
1 ppm ⁻¹ min ⁻¹ = at 298 K, 1 atm total pressure	4.077 × 10 ⁶	4.077 × 10 ⁵	407.7	6.76 × 10 ⁻¹⁶	21.93	1.667 × 10 ⁴	1	164.5
1 m ² kN ⁻¹ s ⁻¹ =	8314 T	8.314 T	8.314 × 10 ⁻³ T	1.38 × 10 ⁻²⁰ T	0.1333	101.325	6.079 × 10 ⁻³	1

To convert a rate constant from one set of units A to a new set B find the conversion factor for the row A under column B and multiply the old value by it, e.g. to convert cm³ molecule⁻¹ s⁻¹ to m³ mol⁻¹ s⁻¹ multiply by 6.023 × 10¹⁷.

Table adapted from High Temperature Reaction Rate Data No. 5, The University, Leeds (1970).

Equivalent third order rate constants

A \ B	cm ⁶ mol ⁻² s ⁻¹	dm ⁶ mol ⁻² s ⁻¹	m ⁶ mol ⁻² s ⁻¹	cm ⁶ molecule ⁻² s ⁻¹	(mm Hg) ⁻² s ⁻¹	atm ⁻² s ⁻¹	ppm ⁻² min ⁻¹	m ⁴ kN ⁻² s ⁻¹
1 cm ⁶ mol ⁻² s ⁻¹ =	1	10 ⁻⁶	10 ⁻¹²	2.76 × 10 ⁻⁴⁸	2.57 × 10 ⁻¹⁰ T ⁻²	1.48 × 10 ⁻⁴ T ⁻²	1.003 × 10 ⁻¹⁹	1.447 × 10 ⁻⁶ T ⁻²
1 dm ⁶ mol ⁻² s ⁻¹ =	10 ⁶	1	10 ⁻⁶	2.76 × 10 ⁻⁴²	2.57 × 10 ⁻⁴ T ⁻²	148 T ⁻²	1.003 × 10 ⁻¹³	1.447 × 10 ⁻² T ⁻²
1 m ⁶ mol ⁻² s ⁻¹ =	10 ¹²	10 ⁶	1	2.76 × 10 ⁻³⁶	257 T ⁻²	1.48 × 10 ⁸ T ⁻²	1.003 × 10 ⁻⁷	1.447 × 10 ⁴ T ⁻²
1 cm ⁶ molecule ⁻² s ⁻¹ =	3.628 × 10 ⁴⁷	3.628 × 10 ⁴¹	3.628 × 10 ³⁵	1	9.328 × 10 ³⁷ T ⁻²	5.388 × 10 ⁴³ T ⁻²	3.64 × 10 ²⁸	5.248 × 10 ³⁹ T ⁻²
1 (mm Hg) ⁻² s ⁻¹ =	3.89 × 10 ⁹ T ²	3.89 × 10 ³ T ²	3.89 × 10 ⁻³ T ²	1.07 × 10 ⁻³⁸ T ²	1	5.776 × 10 ⁵	3.46 × 10 ⁻⁵	56.25
1 atm ⁻² s ⁻¹ =	6.733 × 10 ³ T ²	6.733 × 10 ⁻³ T ²	6.733 × 10 ⁻⁹ T ²	1.86 × 10 ⁻⁴⁴ T ²	1.73 × 10 ⁻⁶	1	6 × 10 ⁻¹¹	9.74 × 10 ⁻⁵
1 ppm ⁻² min ⁻¹ = at 298 K, 1 atm total pressure	9.97 × 10 ¹⁸	9.97 × 10 ¹²	9.97 × 10 ⁶	2.75 × 10 ⁻²⁹	2.89 × 10 ⁴	1.667 × 10 ¹⁰	1	1.623 × 10 ⁶
1 m ⁴ kN ⁻² s ⁻¹ =	6.91 × 10 ⁷ T ²	69.1 T ²	6.91 × 10 ⁻⁵ T ²	1.904 × 10 ⁻⁴⁰ T ²	0.0178	1.027 × 10 ⁴	6.16 × 10 ⁻⁷	1

See note to table for second order rate constants.

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4. TITLE AND SUBTITLE Compilation of Chemical Kinetic Data for Combustion Chemistry. Part 1. Non-Aromatic C, H, O, N, and S Containing Compounds. (1971-1982)				
5. AUTHOR(S) Francis Westley, John T. Herron, and R. J. Cvetanović				
6. PERFORMING ORGANIZATION (If joint or other than NBS, see instructions) NATIONAL BUREAU OF STANDARDS U.S. DEPARTMENT OF COMMERCE GAITHERSBURG, MD 20899			7. Contract/Grant No.	
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